Molecular Modeling with Augmented Reality (MMAR): An Educational Web System for the Learning of Molecular Structures

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Abstract

Learning about molecular structures often becomes abstruse, due to its complex compositions, being aggravated by the restricted interactivity provided by the software commonly used. This difficulty can also be attached to the fact that most students do not present the necessary knowledge to work with biomolecular systems, affecting also the motivation in the object of study. In this context, the objective of this work is to analyze the influences related to interactivity, usability and motivation, provided by a web system called MMAR (Molecular Modeling with Augmented Reality), designed to support the learning of three-dimensional (3D) molecular structures. The system was applied to twenty-five students in the Chemistry discipline, from a technical course in a public school from basic education in Brazil. The results show that it was possible to assist students in the gain of knowledge, while simultaneously allowing them to enjoy themselves, providing unconventional learning, by increasing attractiveness, curiosity, attention, enthusiasm and relevance of such a complex subject in Chemistry.

Keywords: *Molecular Modeling; Augmented Reality; Teaching and Learning; Web System.*

1. Introduction

Information and Communication Technologies (ICT) have transformed the methods adopted by education into more interactive and accessible ones (RAHMAN et al., 2016), allowing the emergence of new paradigms of teaching and learning. One of these technologies is the Augmented Reality (AR), whose application has enabled numerous solutions to be developed for the educational field, providing impacts of great relevance (SILVA et al., 2016).

AR technology changes the human-computer interaction, by providing new learning interfaces that inevitably alter the study environment (IWANE et al., 2016). As it enables the simultaneous coexistence of real and digital worlds (BRONACK, 2011), researchers are increasingly exploring the potential of this technology (WU et al., 2013), in areas such as Chemistry, Mathematics, Biology, Physics, Geography, among others, both in basic and higher education (LEE, 2012). In the field of Chemistry, it stands out as a tool more specifically related to 3D molecular modeling.

Due to the complexity of chemical structural compositions, learning about molecules often becomes abstruse. Another problem is directly related to intuitiveness and interactivity in relation to existing 3D models, since many are limited in detail realism and are not always intuitive enough for users to properly extract information and/or conclusions. As an aggravating factor, interactivity is restricted in most cases to movements and simple actions, such as rotation, translation, color and texture change, being predominantly performed by means of standard peripherals, such as mouse or keyboard (MAIER; KLINKER, 2013a). In addition, these peripherals become barriers both to the ease of manipulation of molecular structures and to the user's own interactivity with them. Thus, in accordance with Essabbah, Otmane and Mallem (2008), the exploration and interaction in existing virtual molecular modeling environments are often simplistic and limited, evidencing the absence of a strong 3D natural interaction.

In this context, a typical problem faced by students is to relate apparently artificial molecular visualization to the normal 3D world, which is even more striking since students do not normally have the knowledge or the abstraction expertise necessary to work with biomolecular systems (NICKELS et al., 2012), also affecting their motivation. In this scenario, a research question arises:

- How to provide technological and educational resources that allow students to learn 3D molecular structures in a more intuitive and motivating way, contemplating interactions with more realistic virtual models, which are performed by more natural means than the traditional ones?

Looking to answer this question, this research proposes the creation of a web system, which uses an AR interface for 3D molecular modeling, seeking to provide the learning of molecular structures with more realistic virtual models, by interaction means more natural than the traditional ones. The final objective is to increase the students' interest in the contents related to the molecules and, consequently, in the discipline of Chemistry. Thus, we analyze the influences related to interactivity, usability and motivation, provided by the environment. The article is organized as follows: in Section 2, teaching and molecular modeling are addressed; Section 3 gives a brief overview of AR technology and 3D molecular structures; in Section 4 the related works are presented; Section 5 describes the research method, detailing its steps; in Section 6 the results are analyzed; Section 7 discusses the results, closing in Section 8 with the conclusion.

2. Teaching and Molecular Modeling

The difficulty of understanding molecular structures is part of the reality of students and teachers. According to Maier and Klinker (2013b), this can occur due to the fact that they have difficulty in imagining the spatial structure of the molecules, since a two-dimensional representation is usually used through slides presentation or the blackboard itself. And, if one student does not obtain the 3D understanding of the chemical structures, it will be very difficult for him/her to understand certain molecular behaviors. Thus,

3D virtual models of a particular molecule can be used to understand, explore and analyze their chemical structure more precisely. This process will allow the visualization of the elements forming this structure, of the different types of bonds between atoms and their angles, and also of their surface.

In this sense, the 3D visualization of molecular structures plays a crucial role to understand the various concepts related to it. Consequently, tools which enable the generation of virtual molecular models are of great importance in education (GOBERT et al., 2011), since these models can help students in understanding theories, phenomena or rules, and also illustrate or simplify abstract concepts (BODE, 2016). According to Badi'Abdul-Wahid et al. (1990, p.1), "molecular modeling is a field that traditionally has high computational costs". However, Bokhari et al. (2002) justify that this is an important tool for the investigation of the collective behavior of systems resulting from the complex interactions between their individual components. Awasthi and Sharma (2012) complement, affirming that it is an essential instrument to understand practically all biological phenomena, since it provides a direction for theoretical interpretation of the structure-activity relation. In this field, several representations have been adopted over the years to work with abstract molecular models, such as stick, space filling and CPK models (HARRISON et al., 2013), which allow 3D representations of molecular structures and are interactive, thus playing an important role in both teaching and learning (LEACH, 2001).

3. Augmented Reality and 3D Molecular Structures

Augmented Reality is an emerging technology that seeks to digitally merge the "everyday world", making possible to produce digital objects in the real world as if they were real objects (LIBERATI, 2015), which occurs by inserting virtual objects superimposed or combined with the real world, improving the actual image with additional information. An AR system must also enable real-time interaction, and to control both real and virtual objects in the 3D space (MIHELJ; NOVAK; BEGUŠ, 2013). This way, there is a very close relationship between physical and virtual objects, being that the former are capable of being enriched by means of additional information, making this condition extremely powerful to the educational process (CADAVIECO, 2014).

The aim of AR in education is to provide a rich educational experience, with virtual models that are used as learning materials in the real world. These models can provide users with fast and deepened multimedia experience during their interactions with the real-world environment (MAITI; KIST; SMITH, 2016). According to Farias, Dantas and Burlamaqui (2011), AR is a different tool to support teaching activity, as it reinforces students' perceptions and emphasizes information that is not directly perceived by the use of their own senses. Kaufmann and Papp (2006) complement, stating that this use can positively influence the learning process.

4. Related Work

According to Lau, Oxley and Nayan (2012), AR software have been applied in areas such as manufacturing, medical, tourism, gaming and education. In the educational field, it allows the addition of contextual information, which improves understanding, especially in more abstract areas as molecular biology. Some

systems have already been developed with the proposal of working with molecules through this technology, seeking mainly the ease of use, which as pointed by Nielsen (1993), makes the development of a certain work more satisfactory, even if performed by an inexperienced user.

Among these systems is Educ-AR, proposed by Farias, Dantas and Burlamaqui (2011), which allows the teacher (end user) to create and save classes using AR, without the need to have knowledge in programming, AR applications or 3D modeling. Another system is ProteinScanAR which was developed by Nickels et al. (2012), having as specific objective its application in molecular biology at high school, with the intention of allowing the creation of classes using simple methodologies, but having the differential of being more intuitive and, consequently, more attractive.

Maier, Klinker and Tönnis (2009), by their turn, present a system not only directed to the work with traditional molecular structural models, but also representing chemical reactions between the molecules. The system is called Augmented Chemical Reactions and seeks to increase understanding and facilitate learning of chemical reactions by visualizing and controlling 3D virtual models of molecules in an intuitive way. Finally, the work of Singhal et al. (2012) presents the construction of a system to provide an efficient way of visualizing and interacting with molecules, allowing a better understanding of the spatial relations between them, as well as the chemical reactions.

This research differs from the works mentioned by performing an analysis, focusing on the influences related to interactivity, usability and motivation perceived by students, provided by means a differentiated web system that allows the creation of complete lessons using AR for the teaching of 3D molecular structures.

5. Method

Regarding methodological procedures, this study has a mixed methods approach (qualitative-quantitative). As for the objectives, it is an exploratory research, which according to Zikmund (200) seeks to develop and apply studies that are indispensable to diagnose situations, explore alternatives or discover new ideas.

In this research, five lessons were elaborated and applied to two group of students using the web system called MMAR - Molecular Modeling with Augmented Reality (Mazzuco, 2017; Mazzuco et al., 2018), which was designed and developed to support the learning of 3D molecular structures using Augmented Reality. The study is divided into four main steps, which occurred between June and July 2017.

5.1. Step 1 - Research Scope

The research took place in the context of a technical course (Events Technician) integrated to basic education in a public school from Brazil. Initially, a meeting was held between the teacher of the Chemistry discipline and the researchers, contemplating the contextualization of the MMAR project and the proposal of the system application to one or more classes of the course.

In a new meeting, at the following week, it was demonstrated the practical use of the system, where it was exemplified the registrations of molecules, users, lessons, etc. At this meeting, the teacher proposed that the approach could be undertaken for two distinct classes, and it would cover the subjects presented in previous lessons taught by him. Thus, the teacher created five lessons in the MMAR system, adapting the

content previously presented in a conventional manner in the classroom, including the same molecules. Each lesson was planned to have 45 minutes of duration.

5.2. Step 2 - Creating the Lessons in the MMAR System

The MMAR system is a project that focuses on lessons management, empowered with AR technology for working with molecules. It requires authentication to be accessed and allows the user of the category "Administrator" to manage it completely, including the registration of users from categories "Teacher" and "Student". Each "Teacher" is allowed to manage "Groups" (classes), these being students (users previously registered), and is responsible for registering "Molecules", linked to certain categories previously registered (such as "Amino Acids", "Proteins" and "Viruses").

At the registration of a "Molecule", it is possible to inform data about it, such as category, descriptive summary, organism belonging (if it is a protein, for example), full description and image. To enable the use of the AR interface it is necessary to upload an X3D file (the widely used open standard for 3D content distribution), containing the spatial descriptions of the structure. Free and scientifically-oriented software for visualization and molecular modeling, such as VDM and Chimera, easily allow the exportation of such objects (molecules) to the X3D standard, which facilitates access to these files.

In the context of this research, the creation of lessons in the system followed the steps below:

a) User registration: initially the teacher created individual users for each student, which in turn were divided into two groups (classes): Class A with 11 students, and Class B with 14 students.

b) Registration of molecules and assignment to lessons: 21 molecules with their respective descriptions, images and X3D files (exported by the VDM software) were registered. Firstly, with the selection and adaptation of the content in the system, three lessons were created, named: "Organic Chemistry", "Sulfur Compounds – Tiocomposites" and "Sulfur Sulfonic Acid Compounds".

In order to demonstrate the complexity of analyzing larger molecules (with a large number of atoms), two extra lessons were added: "Zika Virus" and "5MR3 Protein". As they were not contemplated in the subjects foreseen in the discipline of Chemistry, they were denominated as being "extra". Thus, just a brief contextualization (such as the origin of the molecule, number of atoms, etc.) was carried out in the lessons, with a reduced working time of 15 minutes for each.

Table 1 shows the information related to each lesson: the topics of the discipline discussed, the workload, and examples of molecules linked to each lesson.

Table 1. List of lessons created in the MMAR system (Source: the authors).

Lesson	Topics	Workload	Examples of Molecules
Organic Chemistry	Nitriles, Isonitriles, Nitro compounds and Organic Halide	45 min	1,3,5-Trinitrobenzene, 4-Methylnitropentane, Nitrobenzene, Nitroethane and Trinitrotoluene – TNT
Sulfur Compounds - Tiocomposites	Thiols, Thioethers, Thioesters, Thioketones and Thiophenols	45 min	3-Ethyl-2,4-Dimethylpentane, Ethyl benzoate, Methyl benzoate, Methyl propanoate and Sufenil propene thiol
Sulfur Compounds - Sulfonic Acids	Sulphonic Ester and Amides of Acids Sulphonic	30 min	Methanesulfonic acid, Ethanesulfonic acid, Glutathine sulfonic acid, Sulfanilamide and Sulfadimidine
Extra lesson: Zika (Virus)	Contextualization	15 min	Zika Virus
Extra lesson: 5MR3 (Protein)	Contextualization	15 min	5MR3 Protein

List of lessons created in the MMAR system.

With the lessons created in the system, the two classes were linked, allowing the access of its members. Figure 1 illustrates a screen capture of one of these lessons, in the “My Lessons” section (left menu), named “Sulfur Compounds – Tiocomposites”.

Figure 1. Lesson "Sulfur Compounds – Tiocomposites" created in the MMAR system.

As shown in Figure 1, within a lesson the selection of a molecule is enabled. When clicking it, its illustrative image (which allows being enlarged), the complete description and a green button related to the use of the AR interface are presented. By clicking on this button, a new window will open in the browser, activating the computer webcam. Printed markers need to be captured by the webcam for the 3D virtual model to start working.

5.3 Step 3 - Evaluation definitions

The evaluation purpose is to analyze the students' perception after using the MMAR system, focusing on the identification of influences related to the interactivity, usability and motivation aspects. Thus, an instrument was constructed, with components for each of these aspects, described as follows.

a) Interactivity: an adaptation of the guidelines proposed by Silveira and Carneiro (2012) is made, composing five closed questions.
b) Usability: an adjustment in the questionnaire proposed by Rezende (2013), which focuses on the evaluation of educational software for science teaching, is made, resulting in five more closed questions.
c) Motivation: part of the questionnaire suggested by Savi (2011) is applied in an adapted way, composing the five final closed questions.

Table 2 shows the 15 closed questions of the evaluation instrument. Each one has the 5-point Likert scale response options, ranging from -2 to +2 (Strongly Disagree, Somewhat Disagree, Neither Agree nor Disagree, Somewhat Agree and Strongly Agree).

Table 2. Questions that compose the evaluation instrument.

Item	Interactivity
1	The system provides easy-to-remember forms of use/interaction, not excluding the need for accessible instructions.
2	The system uses resolution and format of images and videos compatible with the available in the web.
3	The system cares not to have visual effects that may hinder user interaction, focusing in what matters (learning).
4	The system uses menu options, buttons and navigation links clearly standardized and consistent with the other interface features used in the system.
5	The system always maintains a standardization of layout (colors, fonts, images, etc.).
	Usability
6	It is easy to learn how to explore and use the different modules and activities of the system.
7	It is easy to use the system.
8	The characteristics of the system (standardization of screens, navigation, design, etc.) make it easier for the user to memorize the interaction paths and procedures for proper use.
9	The information contained in the system (for example, relating to lessons and molecules) is presented in an understandable way.
10	The interaction with the system is pleasant and attractive, you feel satisfied.
	Motivation
11	The design of the system is attractive.
12	The variation (of form, content or activities) helps me to keep the attention in the system.
13	The content of the system is relevant to my interests.
14	The content of the system is connected with other knowledge I already had.
15	It was easy to understand the system and start using it as study material.

Items that compose the evaluation instrument used in this research.

To give the students greater flexibility at the moment of evaluation, not remaining limited to the closed questions, in addition of these items two open questions were included at the end of the instrument: “What

would be the strengths of the system?" and "What would be the suggestions for improvement of the system?".

5.4 Step 4 – Experiment conduction

The experiment was conducted with one week interval between the two classes, with the exact same procedure. The students arrived at a laboratory containing 15 all-in-one microcomputers, with only one student per computer.

Firstly, the teacher made a brief explanation of the experiment, relating it to the Chemistry lectures that were given. Then, students received instructions regarding the activities that should be performed and were invited to access the MMAR system on the Internet, being directed to the "My Lessons" section.

Students were free to explore the content of each lesson as well as to manipulate any molecule through the AR interface, as shown in Figure 3. While using the AR interface, students were asked to answer queries such as: "List the organic functions of this molecule", "Identify the functional groups present in this molecule", "Write the molecular formula of the compounds of this molecule" and "Write the name of the compounds that present only one functional group".

Figure 3. Students using the MMAR system.

Likewise, students were able to access the extra lessons, which exemplified the manipulation of molecular models of greater complexity. After the activities, students were asked to logout the system, turn off their computers, and to individually respond to the evaluation instrument, which was made available in printed form. For this moment, students were encouraged to reflect on the activities just performed, as well as to evaluate the system in a sincere and spontaneous way, regardless of whether their perceptions were considered good or bad.

6. Data Analysis

In this section, we present the analysis of data obtained from the experiment application, organized according to the aspects evaluated.

6.1 Interactivity

Figure 4 shows the graph containing the values (percentages) corresponding to each question of this component, in relation to the five Likert scale alternatives, highlighting that none of the assertions received "Strongly Disagree", "Somewhat Disagree" or "Neither Agree nor Disagree" answers.

Question 1 received the best evaluation of this component, containing 84% of the ratings attributed to the "Strongly Agree" and 16% to the "Somewhat Agree" response, demonstrating that the system has features focused on simplicity, objectivity, visual consistency and clarity. Question 2 had 64% of the ratings directed to the "Strongly Agree" option, and 36% to the "Somewhat Agree" response, confirming that the system uses a resolution and a format of images and videos compatible with the web.

Question 3, on the other hand, is the one that presents the lowest percentage of evaluations attributed to the "Strongly Agree" response, with 56%, as the other 44% were given to the "Somewhat Agree" option. However, it still represents an excellent evaluation for this issue, allowing to infer that the system contemplates features such as design free of irrelevant information, prioritizing aspects regarding cleanness and clarity of the graphical interface.

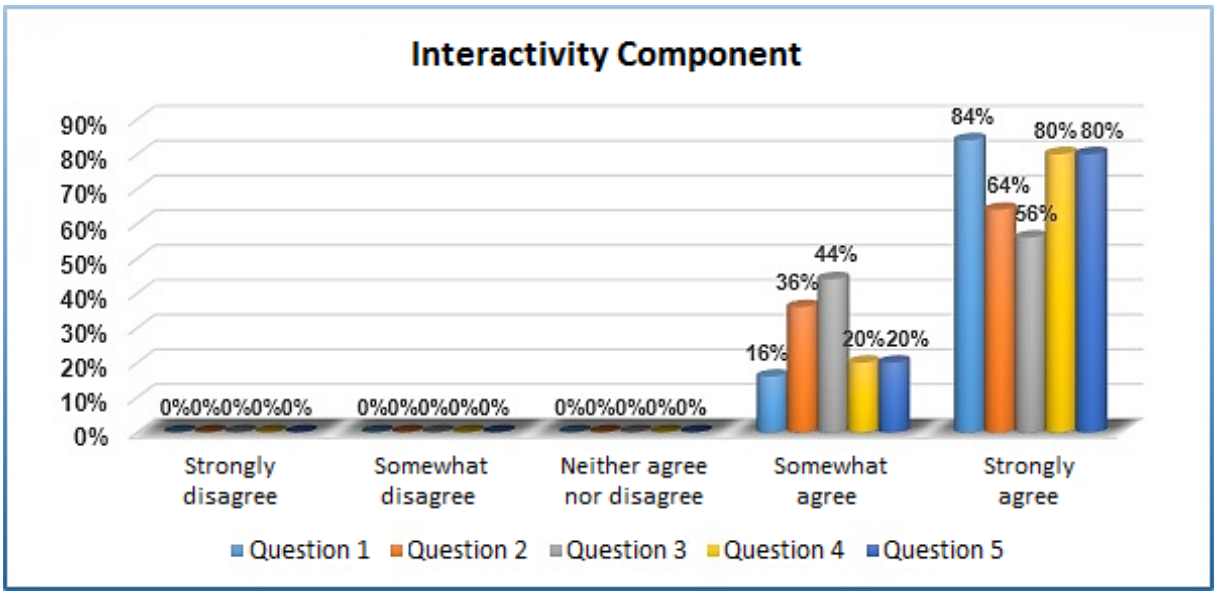

Figure 4. Results for the Interactivity component.

Question 4 received 80% of the ratings for the "Strongly Agree" response, and the other 20% to the "Somewhat Agree" option. These results corroborate that the system presents good navigation characteristics, such as appropriate colors and visual elements that maintain the interfaces and are compatible with their functions. Question 5 presents the same ratings, reinforcing results that indicate that the system has a visually standardized layout, including clear and objective messages.

6.2 Usability

Figure 5 outlines the graph covering the values (percentages) corresponding to each question in this component, for each of the five Likert scale alternatives, indicating again no presence of "Strongly Disagree", "Somewhat Disagree" or "Neither Agree nor Disagree" answers.

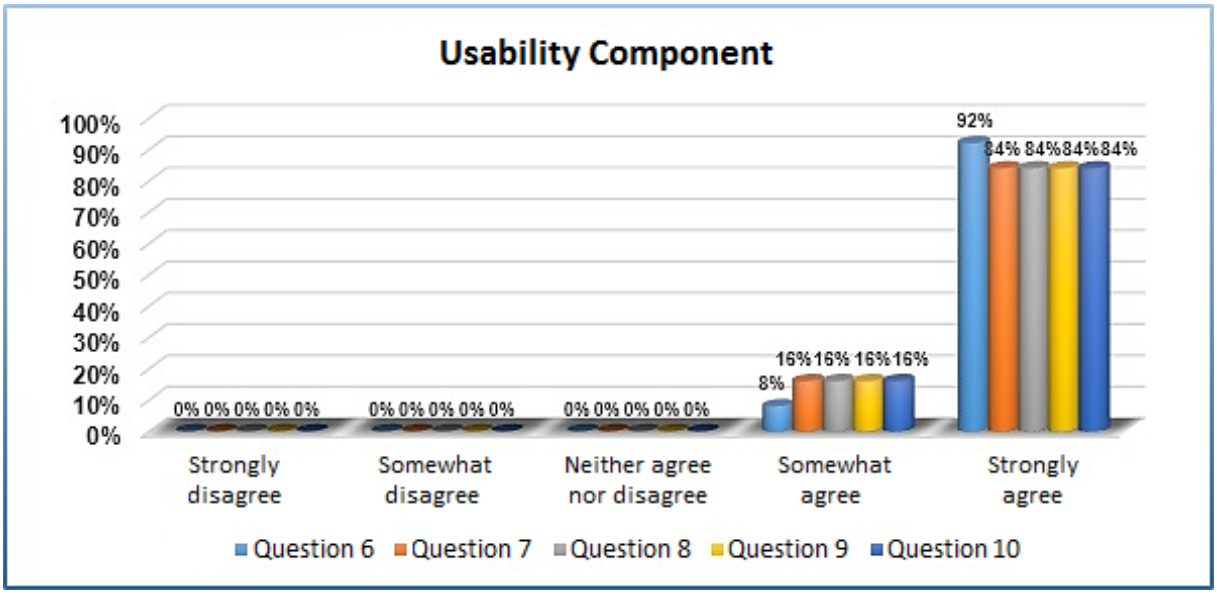

Figure 5. Results for the Usability component.

Question 6 presents the highest percentage value (92%) directed to the "Strongly Agree" option, not only in this component, but also among all the questions of the instrument. This value expresses an important feature of the system regarding the ease of learning: it enables the user, who is accessing for the first time its graphical interface, to learn it enough to carry out the necessary basic tasks.

Questions 7 to 10 present the same rating percentages: 84% of answers to the "Strongly Agree" and 16% attributed to the "Somewhat Agree" option. They refer to the system ease of use (efficiency), considering aspects related to users' experience, as their physical and cognitive effort during the interaction process, as well as the speed and the number of errors during the execution of a given activity. These results reflect the system support to user memorization, by improving the standardization (considering the harmony) of all elements of the graphic interface, such as colors, fonts, menus, links, forms, etc. Also, it contemplates aspects related to users' satisfaction, a subjective condition to which they consider the interaction with the application pleasurable and interesting.

6.3 Motivation

Figure 6 illustrates the values (percentages) corresponding to each question of this component, according to the five Likert scale alternatives. It can be observed the presence of a slight disagreement and neutrality of answers, which did not occur in the previous components.

Question 11 presents a percentage of 84% for the "Strongly Agree" response (the highest in this component), with the other 16% attributed to the "Somewhat Agree" option. These values show that students considered the graphical interface attractive. They in fact mentioned that the system is interesting, considering it a "light" environment, and enjoyed the diversification of the sections. However, the attractiveness of the AR interface was notoriously outstanding in relation to the other interfaces presented by the system.

Question 12 obtained a percentage of 80% of evaluations directed to the "Strongly Agree" response and 20% to the option "Somewhat Agree". This result allows to infer that the system is able to make the user stay attentive, not only because of the content variation (classes, molecules, etc.) or the activities created by the teacher, but also by the characteristics of the graphical interface presented by the system itself.

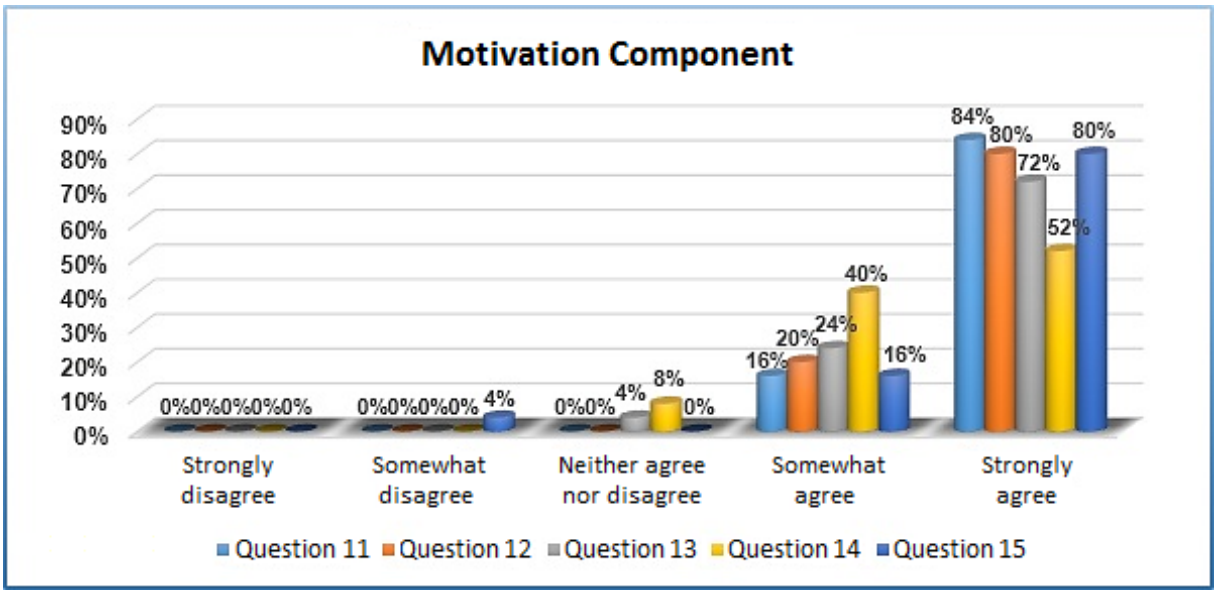

Figure 6. Results for the Motivation component.

Question 13 was the first one to expose percentage values that deviate from the standard presented by the questions analyzed so far. It shows a percentage of 72% of the ratings attributed to the "Strongly Agree" response, and 24% addressed to the "Somewhat Agree" option, but 4% to the "Neither Agree nor Disagree" response. This fact can be related to the understanding of the question (which is extremely subjective). Also, as during the experiment some students commented that "they did not like Chemistry", there is possibly a relationship between a student "not liking Chemistry" with the degree of relevance of the content presented by the system to their interests. However, noted that this value corresponds to just one respondent, this result demonstrate that overall the system has successfully fulfilled the goal of being relevant to students' interests.

The values presented by Question 14 are similar to the previous question. A percentage of 52% of the answers were directed to the "Strongly Agree" option, 40% addressed to the "Somewhat Agree", and 8% to the "Neither Agree nor Disagree" response. This question also presents the lowest "Strongly Agree" rating among all questions of the three components of the instrument (52%). On the other hand, it also presents the highest "Somewhat Agree" percentage of answers (40%). Thus, this result shows that the system reached an excellent average in this point, allowing to verify that it contemplates the aspects that involve the connection of the content exposed in the system with other knowledge that the user holds.

Question 15 presents a percentage of 80% to the "Strongly Agree" response and 16% attributed to the "Somewhat Agree" option. However, this was the only question that presented a value for the "Somewhat Disagree" response (4%). Overall, this result portray the satisfaction of the students, being related to the ease of understanding provided by the system features. The disagreement may have occurred by an

imperfect interpretation of the statement by the student, corroborated by his positive comments in the open question regarding the system: "It is very cool and different. The design is very good and easy to access".

6.4 Open Questions Analysis

In this section, clippings of the most relevant answers given to the two open questions are presented *ipsis litteris* and analyzed. First, it is worth noting that all the students answered these questions, and it was observed that they showed interest in responding it according to what they actually considered about the use of the system, allowing the collection of real answers, without the influence of the teacher or the researchers. The first question analyzed is: "*What would be the strengths of the system?".*

In relation to aspects consistent with the Interactivity and Usability components, the respondents reported that: "the standardization of the screens facilitates the study"; "easy to access, with surprisingly easy-to-use graphics"; "well organized, understandable and easy to handle"; "interactivity with the proposed subject, clean design, easy to use". These comments are consistent with the answers to the closed questions, especially regarding the possibility of users to easily remember the actions that they need to perform certain activities, the compatibility of the graphical interface elements with its application context, and the consistency of the graphic elements with their respective functions.

Addressing aspects related to the Motivation component, students mentioned: "the system allows a greater understanding of the content"; "the molecules seem attractive and it's an innovative and amazing system"; "it's really cool and different, really interesting to work with"; "it gives me more pleasure to learn and to see molecules of chemistry"; "it facilitates understanding"; "it's interesting, different, and a very clear way of showing us the molecules, a great program, a system with a lot of innovations that draws our attention". The answers given by the students demonstrate that the system satisfactorily contemplated the integration of a technology still underused in the educational scenario. It also addresses the users' subjective pleasure and enthusiasm, which are linked to the ease of comprehension provided by the system's functionalities.

The second open question was: *"What are your suggestions for improving the system*?*"*. The first salient aspect identified in students' comments is related to the content posted by the teacher, since they mentioned "update it with more information" and "more content". Thus, although three lessons were created, each with their respective descriptions and illustrative images (as used in classroom presentations), containing a total of twenty-one molecular models that could be manipulated using Augmented Reality, they wanted more. Possibly, this requisition is related to the fact that the system provides an environment in which the student feels pleasure to be involved, corroborated by the answers to the previous question. This result shows that students seek more and more content and molecular models to be manipulated through AR interface, as each model becomes a surprise at the time of its visualization.

The second aspect highlighted is related to the extra lessons, entitled "Zika (Virus)" and "5MR3 (Protein)". Comments were quoted as "improve the functioning with larger molecules", "avoid locking" and "the difficulty of loading some molecules". However, the teacher informed the students during the experiment that some molecular models belonging to the two mentioned lessons were larger, and that, because of that, their download would possibly take longer than the others. Also, that there would be the risk of blockages, because the processing of these models would be requiring more from the system.

The third aspect identified in students' comments is directly related to the type of molecular models used, since they mentioned that "it could expand to visualize the bonds inside the molecule" and the need for "colored subtitles with the name of the molecule". Nevertheless, deployments of these suggestions rely solely on the software used to generate X3D files, which have to support such requirements. For example, if a certain software supports the visualization of the bonds or the subtitles, it takes only to export the model containing these characteristics and importing it into the MMAR system.

7. Discussion

In light of the obtained data, it is possible to observe the effects of the system application to the learning of molecular models, especially regarding the aspects of interactivity, usability and student motivation. The main findings according to each aspect are discussed in this section, confronting it with the students' comments and the knowledge available in the literature.

7.1 Interactivity

The system allows to maintain the same standard form of teaching adopted in the classroom, using texts, images, slides and videos, but adding the interactivity aspect, which allows creativity and curiosity to be aroused in the students, making learning more attractive and dynamic. Cadavieco (2014) emphasizes the importance of making use of AR as a complementary and beneficial tool to the educational process, which was verified in the students' comments, such as "it awakens curiosity about the content, facilitates the visualization of the molecules, allows a better understanding of the matter" and "it allows to better visualize the formulas of the molecules and to have fun while learning".

The results for the Interactivity component allow us to ratify the heuristics of Nielsen (2003), regarding the possibility of the user to easily remember the actions needed to properly perform the operations, without having to consult instructions or any kind of manual, regardless of the time interval without interacting with the system.

According to the results, the premise of preventing the system from having visual effects that would make it difficult to interact, diverting the user attention from what really matters (learning from interactivity), was contemplated. Also, the condition proposed by Silveira and Carneiro (2012), which seeks to provide that the user can interact without the focus being lost and, likewise, prioritizing the compatibility of the graphical interfaces elements with their respective application contexts. In addition, by making use of standardized menu options, forms, buttons and navigational links, the system proves to be committed to the idea of consistency presented by Nielsen (2003), in relation to the ease of learning, taking less time and effort for users to reach a certain level of familiarity with the system.

7.2 Usability

Although the numerous resources available, the system was considered simple, objective, and easy to use and to understand, presenting a more natural way of manipulating molecular models, making students more interested in the content. These aspects can be observed by means of the results for the aspects evaluated, as well as in students' comments, as "excellent resolution and understanding of the system", "interactivity

with the proposed subject, clean design, easy use", "better understanding of the subject in an interactive way, stimulating the interest" and "easy access to the system, makes it possible good studies". The ease of learning is in line with Rezende's (2013) proposal, which emphasizes the importance of the easiness offered by the system, with the purpose of allowing the user to explore and to make use of both the different sections (modules) and the different tasks (registered in the system).

On several occasions during the experiment, the students commented out loud that the system was very easy to use, and even though they were using it for the first time, they did not need to access the "Help" button. Thus, it can be observed that the ease of learning is also related to other aspects, such as the guidance and navigation mechanisms employed. In addition, the system respects the heuristic of Nielsen (2003), regarding making users to perform few actions to achieve their goal, facilitating the memorization process and, consequently, favoring the use.

Finally, the system was considered useful in complementing the content seen in the classroom, regarding the Chemistry discipline, allowing students to gain a better understanding of the subjects already studied, and to review already formed opinions and concepts, reinforcing the assumption of Farias, Dantas and Burlamaqui (2011), who admit that AR is a differentiated tool to support teaching activity. This was observed both in the behavior and in students' comments, such as: "So... the TNT molecule is like this!" and "The molecules are very different!".

7.3 Motivation

With the Augmented Reality interface it was possible to motivate students to increase the manipulation (and study) of a larger quantity of molecules, corroborating with ideas from Lau, Oxley and Nayan (2012) and from Kaufmann and Papp (2006), who acknowledge that AR can positively influence the learning process. This can be seen by observing the evaluations for the Motivation component and in students' assertions, such as "great program, a system with many innovations and that draw attention", "molecules are now more attractive and it is an innovative and incredible system", and "it would be interesting to have more molecules".

It was noticed that the system can help the student in the fixation of knowledge, while simultaneously it distracts, providing an unconventional learning, meeting the concepts of Vijay et al. (2016), who state that AR has modified the teaching and learning scenario in an innovative and interesting way. This is corroborated by students' statements, as "it's very cool and different...", "it's more attractive for learning", "easier understanding of the subject", and "learning quite differently".

The responses also portray the success in accomplishing the task of designing and developing a system integrating a technology that is little used in the educational scenario (AR). It supports researches like the one of Rezende (2013), which includes aspects related to users' satisfaction, where they evaluate the interaction as pleasurable and interesting, feeling satisfied with the system; and Nielsen (2003), that addresses subjective satisfaction, which is directly related to the ease of understanding made possible by the system's functionalities.

The knowledge achieved (with the system) was considered by students relevant and useful, allowing them to learn in a playful and pleasurable way. As during the system use, manipulating the molecular models

through the AR interface, users were also studying, the assumptions of Maiti, Kist and Smith (2016) were met, meaning that the use of this technology in education has the potential to provide a rich educational experience, helping in the process of understanding complex subjects. This can also be perceived in the students' comments, such as "it gives me more pleasure to learn and to see the molecules of chemistry" and "it facilitates understanding".

The experiment carried out showed that it is possible to improve both the students' interest and motivation for learning, by providing resources unconventionally, consistent with their "connected" contemporary reality. This inference is based on observations of how much the interactivity, usability and motivation aspects conferred by the system have influenced the attractiveness, curiosity, attention, enthusiasm and relevance, even in of a complex subject such as molecular compositions.

8. Conclusion

The research started from the principle that a web system, which uses Augmented Reality technology for 3D molecular modeling, can provide a better understanding of molecular structures, in a more attractive and motivating way. The focus was on analyzing specifically the influences related to interactivity, usability and motivation, provided by the system.

As a result, it was verified that the MMAR system allows an unconventional form of object visualization, contemplating interactions with more realistic virtual models, these being carried out by more natural means than the traditional ones. As a consequence, it was observed an accentuating interest of the students in the contents of the Chemistry discipline. They were able to learn while, at the same time, they were enjoying themselves, and after all, they considered the knowledge gained to be relevant and useful.

The teaching method explored in this research sought to provide an alternative to the expository class model, emphasizing the introduction of contemporary education characteristics, as dynamicity and the use of innovative technological resources such as AR technology, so present in the students' reality. We have demonstrated the practical implications and possibilities of this approach, such as allowing and motivating students to manipulate (and study) a greater number of molecules.

As future works, we intend to implement the following improvements in relation to the MMAR system:

a) to enable compatibility of the AR interface with mobile devices;
b) to enable more features in the AR interface, that would allow users to modify the presented model, in order to best suit their needs, such as changing color, brightness, opacity, contrast, sharpness, transparency, lighting angle, etc.;
c) to enable filters in the "My Lessons" section, to allow the searching organized by lessons, users, status, title, etc.;
d) to integrate the system with a distance learning platform, such as the MOODLE (Modular Object-Oriented Dynamic Learning Environment), providing the user with a greater number of resources, as chat rooms, forums, file exchange, etc.

Regarding the study itself, as future research the scope of evaluation can be broaden, considering aspects such as accessibility or intelligibility. Also, a new experiment could quantify the indexes corresponding to the increase (or decrease) of aspects analyzed. For example, to measure how much was the variation in the

student motivation before and after the system use. Another essential point in the continuity of this work is its application with different audiences, as undergraduate or graduate students who have in their respective syllabus the study of molecules, approaching not only simple ones but also the ones with more complexity, such as proteins, viruses and nucleic acids.

9. References

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