Touch on Chemistry: Interaction System

Diogo Henrique Caria Fereira
diogocariaferreira@tecnico.ulisboa.pt

Instituto Superior Técnico, Lisboa, Portugal

December 2020

Abstract

The enjoyment players can get from an immersion in a virtual environment is directly related with how interactive the system is. Virtual Reality becomes more common in games and other applications, pointing for the need to improve the use of this technology especially for teaching and learning pur-poses. The game "Touch on Chemistry" is a game for teaching Organic Chemistry, a field combining high number of theoretical concepts with difficulties on its visualization. By employing Virtual Reality, the game facilitates the visualization of those concepts originating a fun and interactive way of learn-ing Organic Chemistry. We aim to improve the interaction system for "Touch on Chemistry" by imple-menting a model where hand figures and gestures are used to perform actions such as moving, rotat-ing, linking, or grabbing objects, with the use of a Leap Motion device in a virtual environment. These new actions were defined based in data collected from testing users/players and from interviews providing information on the needs felt to increase the interactivity of the system. In order to do so, this dissertation focus on the development of an interaction system that makes use of the Leap Mo-tion capacities of recognizing the hands of the users along with the gestures and hand figures they make. The actions the users can make were catalogued in separated interaction modes. The activa-tion of those modes was mapped with the hand figures and gestures the users can make, creating three interaction models: Two-hands activation model, One-hand activation model and Buttons Model. Each interaction model makes a different use of the Leap Motion capacities in a virtual environment. The model One-hands activation was through the execution of 9 different tasks developed. The re-sults on performance and execution time indicated that this model allows the users to perform the necessary actions and complete the tasks required of the interaction system, improving the immersion experience. Further research on the developed interaction models and the difference between them should be done to create new ways to interact with the system.

Keywords: Virtual Reality; Organic Chemistry; Game; Learning; Hand-Free Manipulation; Leap Motion; Interaction System

1. Introdução

Nowadys we face increasingly interactive societies immersed in information and technologies, where simulation systems gain privileged spaces in teaching and learning processes.Some of these processes already integrate virtual reality and incorporate the playful and ammusement nature of games to skills acquisition.

The number of students applying at national contest of access (CNA) for higher education is increasing almost every according to the Portuguese's governmental institution Direção-Geral de Ensino Superior (DGES) [1]. The growing number of students justify the need of new methods for teaching and learning, mostly using IT technologies applied to scientific domains.

Organic Chemistry also presents a challenge in terms of visualization, since most of the contents would benefit from 3D perception, which is absent from common teaching methods.

At the same time, with the VR technology, all sorts of tests are being made to validate its possible benefits in education, with a positive effect described for several areas including also the chemistry area, where the learning results achieved are better than the ones achieved using more traditional teaching methods. While previously, VR immersion would depend on visual and auditory stimulation, new tools are being developed to improve the immersion experience, by implementing more senses to it, like touch and smell.

In this context emerged the game "Touch on Chemistry", which interactive system will be updated in the present project, considering the improvement based in the use of Leap Motion, in order to de-velop a better and more interactive 3D perception tool. This project will then focus on improving the interaction by making use of the capabilities of the Leap Motion sensor to capture and register the hands of the users in a virtual environment, to better captivate the players and possibly increase the effectiveness of the learning process.

The main goal of this dissertation is the development of an interaction system that can improve the Hands-Free Manipulation within the game "Touch on Chemistry", where the player will be able to directly manipulate atoms and molecules. This will be achieved by increasing the quality of the interaction between the player and the virtual environment, along with its components. The immersion experience is obtained from using VR technology paired with a Leap Motion sensor to capture the hands of the users in the virtual environment.

2. Related work and State of Art

Organic Chemistry is a chemistry subdiscipline focused on the study of the structure, properties, and reactions of organic compounds (chemical compounds that contain carbon) [2]. The study of these factors contributes to know and to understand the compound's chemical composition, its formula, its physical and chemical properties, the chemical reactivity and its behaviour [2]. Organic com-pounds constitute most known chemicals, having diverse structures and a large range of applications, being crucial to life on planet Earth [2].

Nowadays there are several programs, academic or commercially available, applied to organic chemistry. They can estimate names according to the nomenclature systems, draw formulas, predict physical-chemical properties and interactions and all the possible information related to each known compound. Doing an overall evaluation of the market is out of the scope of this project.

For the present project, we will consider just the programs used by the group of interest, the teachers and students of Organic Chemistry at IST, in order to include the main features in our game. VR technology dates back from the 60's (since even the meaning of virtual as in "something not physically existing but made to appear by software" dates back from only 1959[3], however, due to the lack of processing power at the time, there was a huge decline of interest. Only in recent years has the interest in the area of VR resurfaced in the consumer market, with the development of devic-es capable of providing a full immersion in a digital environment, such as the Oculus Rift, a Kickstarter project in 2012, with the purpose of providing an affordable high-quality Head-Mounted Display (HMD) to the public, looking for funding and achieving the goal of $250 000 in less than 24 hours [4]. It is this reawakened interest that contributes to a better understanding of what is being called the "second wave of VR development", where a vast amount of products are emerging and flooding the market, trying to implement aspects of the vision of the Ultimate Display [4]. These devices now have better software, better hardware and new technology, like good haptics, eye tracking programs and better HMD's, along with new applications, such as in training, learning, immersive collaboration, data visualization, retail and gaming [5].

The current version of the game "Touch on Chemistry" was developed using Unity Version 5.6.5f1 and consists of a VR environment simulating a chemistry classroom. For the user to be able to play it needs an HTC Vive with Leap Motion and the setup made through SteamVR. The game main components are objects that represent atoms and bonds. The molecules are the junction (parent) made of the atoms and the bonds between them.

The principal interaction happens when user grabs an atom, which highlights the atom, to make it easier for the player to understand that he is now holding it. The user can grab up to two atoms at a time, one in each hand, since it is not possible to have two atoms held at the same time in just one hand or, an atom being grabbed by both hands at the same time.

Each atom has the number of bonds it can have defined and according to its number of electrons (which is the number that defines the amount of bonds an atom can have [6]). A molecule can be infinitely built by adding more atoms to it, however, two molecules could not be joined together. In the same way, it is not possible to have a circular bond, rings, in the molecule. The game has different game modes implemented, and also the possibility to implement even more. At the present, the ones already implemented are the Normal Mode and the Speed Run Mode. In Normal Mode, players go through the levels by completing the challenge in each of them and trying to get as high of a score as possible. In Speed Run Mode, the purpose is to complete the levels as quickly as possible. Some additional modes that can be implemented are the Building Mode (for the player to creatively build the molecules he wants), the Complete Mode (where the players are given an incomplete molecule and he needs to complete it to pass the level), Transform Mode (a mode for the player to transform one molecule into another) and Multiple Choices Mode (in this mode, the player needs to choose a correct answer based on the provided possibilities). The game also has implemented a Scoring Board, in other to give scores to the performance of the players. To foresee the expectations of the target audience, we conducted a semi-structured interview with two teachers and one researcher from the area of Organic Chemistry at IST. Both teachers had previously played the actual version of "Touch on Chemistry", while the researcher did not.

All interviewed mentioned the importance of having the ability to rotate the molecules. Although it was mentioned that the size of the bonds between the atoms are fixed, it was also pointed that could be useful to stretch the bonds, as such, further inquiry is required for this aspect. Considering the size of the atoms,

all the participants mentioned that hydrogen should be smaller than the other atoms but, there is no need to create further size distinction, since all atoms also have colours to differentiate them. The importance of the geometry in each molecule was mentioned, so additional research should be considered for this matter. Both professors noted the impossibility to join two different molecules and make rings with the atoms as a problem and something that is essential to do.
It was noted that the game should be able to read molecules data from specific files, similar to what they have in other programs frequently used, such as ChemDraw. In the current version, only the levels of the game are reed from a file.
The development of Virtual Reality technology is allowing for an increased diversity of experiences in different areas like entertaining[7][8], training [9] and education[10]. More specifically, using VR has advantages like encouraging learners to experiment by interacting with the environment, providing a multimodal interface to resources supporting learning and allowing the learners to actively participate in the creation and organization of their learning environment This advance of technology and VR techniques is accompanied with newer and better devices, has can be seen with the addition of touch, which became a possibility after the boost in the development of haptic interfaces in 2016 [11]. A different type of hand-based object manipulation device is Leap Motion. So far, all previously listed devices evidence the need to hold a physical equipment in the hands to interact with the virtual environment. However, the interaction provided by the Leap Motion tracks the hands of the person, allowing the user to input the movements and figures of the hands into the virtual environment [12].
Since this device is based on tracking the hands, it is possible for these readings to not always be as precise as it would be intended, which has been verified in several system. On the other hand, this also opens doors to the development of fun and interactive games, with a much deeper degree of immersion, and interactivity.
In the development of this work, it was possible to conclude that VR is a ground-breaking medium with major advantages over traditional visualization and that animated simulations can be made to help users visualize temporal datasets. The interesting point of this conclusions is that, although the focus here was in Biology, it is possible to extract some information for my work, like the use of animations, and the importance of making good use of the advantages of having a VR environment for the display.

3. Metodology

To reach the defined objective of implementing an improved version of the interaction system of the game “Touch on Chemistry”, this project focuses on developing and exploring different ways of inter-action between the users and the virtual environment.
The overall approach of present project will essentially follow an experimental methodology orga-nized in 3 major steps:
STEP 1: Analysis of the pre-existing version of “Touch on Chemistry”; Identification and assess-ment of needs of the users for the new implementation-
STEP 2: Development and Implementation of the System
STEP 3: Validation of the System
For the Step 1 we start by gathering information. The samples are of convenience with volunteers being recruited at the University or online, and when applied, the volunteers signed an informed con-sent (Annex A). We will realize tests of the current version of the system with users from high schools since they are a target audience of the game. This will allow us to gather data on the current perfor-mance of the game. We will also conduct an interview with teachers and researchers of chemistry at university, to know what type of interaction this system is expected to provide and how they would expect this interaction to happen. To better define the interaction possibilities of the system a new set of tests were carried out online with others volunteers.
After gathering the data, it is necessary to analyse its contents in order to identify the aspects that can be improved in the system and its interaction.
Step 2 starts based on all the information previously obtained, by designing possible ways of inter-action. We then develop and implement new interaction models of the system. When the implementa-tion of such models is over, we will proceed to test the system and discuss the data collected from such tests.
For this Step 3, users to test the new system are volunteers and will also sign an informed consent. This validation will be based on time and performance metrics, so the results will evidence if the inter-action is fulfilling the defined objectives or not.
Having finished all the testing and discussion, we will present the conclusions reached by this project. The virtual immersion can be achieved by using a HMD with VR Sensors. For the software, we will use Unity3D, Version 2019.1.11f1 on Windows to create the virtual environment and the SteamVR packages to

allow the connection between the HMD and Unity. For the hands recognition, it is used the Leap Motion device from Ultraleap with the Orion software version 4.0.0 of its Developer Kit and the package of Leap Motion Unity Modules version 4.5.0.

4. Previous Version Data Collectio

To update the system with a new version of the game “Touch in Chemistry”, it was crucial to identify users expectations, as well as to know the performance of the previous version.

We first performed an interview with teachers and researcher of the chemistry department of the “Instituto Superior Técnico” of the Lisbon University. From this interview it was clear that the system should be useful for both classes and autonomous study of students of chemistry. The system was also expected to allow the ratation of molecules, have a good way to control the distance of the links between the atoms, and change the size of the link (if it was a single link, double or a triple). It was also pointed by the interviewed the importance of being able to connect any atom of a molecule or even join two molecules, aspects not working in the previous version.

The first set of tests were held during the activity ‘Laboratórios Abertos DEQ 2020’ [13] through the course of 3 days. A total of 120 highschool students were recruited as testers, of which 55 (45,8%) were men, 21 (17,5%) were women and 44 (36,7%) did not register their gender. Of the 120 users, 66 (55%) had some experience with VR and for the remaining 54 (45%) this test repre-sented their first contact with this technology.

After the test, users answered three questions: “Did you have any struggle while interacting with the system? If so, what was it”, “What did you enjoy the most about the system?” and “Is there any-thing where you think the system could be better?”.

From the answers to those question, we detected that the aspects that required more attention were the performance of the system, difficulties with the mechanic of grabbing the atoms. It was also registered that the creativity and the hands-free interaction was very benefictial characteristics of the game.

The last data set was gathered from video recording of users. It was asked online for universitary users to record themselves performing a certain set of tasks related to the grabbing of atoms and linking of structures. The information from these recording allowed to have an idea of gestures and figures the users would be expected to make with their hands while interacting with atoms.

5. System update

The update of the system was developed in a virtual environement using a Head-Mounted Device and a Leap Motion sensor. By using Unity3D to create the project and the SteamVR unity package and Leap Motion Unity Modules, it was possible to have an environment that detected the movements of the head of a user and his hands. From the SteamVR package we imported the LeapRig prefab, to allow the capture of the user, and to allow the interaction we used the Core Module and Interation Engine unitypackages from the Leap Motion Unity Modules.

The interaction in the game allowed the user to grab atoms, move them, link them, move molecules and rotate molecules. For our project we catalogued this and other actions in interaction modes, seen in table 1.

It is possible to activate Free Mode and Selection Mode from every other state. From the Selection mode, users can choose to activate Translation Mode, Rotation Mode or Link Mode.

Considering how to implement the activation of the new modes by making the most use of the Leap Motion, the solution was to use the recognition of a Hand Figures as activation of a mode, and then a Gesture for performing an action of the mode. The mapping of the Hand Figures to the activation of an interaction mode will be mentioned further ahead.

Designing user interfaces assume as relevant to give feedback to the user about the actions exe-cuted. In our interface system, the feedback is assumed as a change of colour of the hands whenev-er a mode is being activated. By deactivating a mode, the colour returns to the previous one.

Three different interaction models were developed in the upgraded version of the interaction system. These Interaction Models are responsible for mapping the Hand Figures the user does to do the acti-vation of Mode of Interaction.

The first interaction model (Two-Hands Detection Activation) is based on having both hands in a certain position while doing a specific figure in order to activate a mode.The biggest advantage of this model is taking full advantage of the virtual environment around the user to map the selection of the modes. At the same time, it is necessary to consider that this model needs to interpret the Hand Figure of both hands correctly, as such, it can be more frequent for an activation process to stop midways because the Leap Motion misreads the hand figure of one hand.

Table 1: Modes of Interaction of the System and respective description

Mode	Description	Interactions
Free Mode	The player can grab and move the objects, as well as collide them to create new links or remove existing ones.	Grab Object Move Object Collide Objects
Selection Mode	Touching an object selects it and all the objects he is linked to it, either directly or indirectly. If the objects are already selected, they are instead unselected.	Touch Objects
Translation Mode	Translates all selected objects by moving hands.	Move Hand
Rotation Mode	Rotates all selected objects around the center of their links by rotating hands.	Rotate Hand
Link Mode	Allows the player to change the number of links between two objects or remove a link between them.	Pinch Links Cut Links

Each activation is based on the figure of both hands and the position in relation to themselves, however, it should never be with both hands touching each other since that could cause incorrect readings from the sensor of the Leap Motion.The position would consider if the hands were facing each other or the camera. Lastly, the hand Figure of both hands would also be a factor for the activation of the desired mode.

The second interaction model (One-Hand Detection Activation) is similar to the previous one, but only considering the Hand Figure of one hand and the direction it is facing. This interaction model is based on usability and simplicity.By making full use of the aspects of being in a virtual environment with a Leap Motion sensor, using only one hand allows as a controller makes it easier for the user to learn the system controls and the necessary Hand Figures to activate the modes he wants. For this interaction model, whenever the user wants to activate a mode, it is required to look at the palm of the hand in which he wants to activate it. Since the interaction is based only on one hand at a time, once the user starts activating a mode using any given hand, that hand becomes the currently interactable hand, and the user can no longer activate any mode with the other hand until the currently activated mode is deactivated and back to being Free Mode. Something necessary to consider while implementing this interaction model is that, due to the pos-sibility of the Leap Motion incorrectly reading the Hand Figure at a given time, this could activate a mode when such is not intended. To correct those misreadings from the Leap Motion, it was neces-sary to implement some extra factors, which were the need to face the camera when doing a Hand Figure and to wait for a small amount of seconds.

The last interaction model implemented was based on buttons.(Buttons). As previously stated, the Leap Motion does not always make the best capture and reading of the hands. As such, in this model, the selection of modes involves pressing a button in a UI panel next to a hand to activate a mode. After a button was pressed, the user would need to put one of his hands in the specific Hand Figure associated with the desired mode activate it. The Hand Figure are the same ones used in the previous model. Pressing buttons are actions with large familiarity and infallibility in the perspective of the individuals, due to social technological advancements, as such, by using a model based on buttons, it would be clear for the user what action is needed. The combination of buttons and hand figure capture increases the accuracy of this model to activate modes, avoiding the chance of a mode activation being triggered by accident from an incorrect detection of the hands figure.

To validate the interaction system developed, it was also implemented a testing system. To have the testing system be fully operational and as autonomous as possible, it was necessary to introduce the tasks into the system as a custom data type.

6. System Analyses

To test the quality of the implemented interaction system we organize a set of tests To ensure minimal intervention between the investigator and the tester as possible, it was also added to the scene an instruction board clarifying the instructions about the fingers to ac-tivate each mode. The choice of this model as the only one to be tested is justified by its simplicity and usability assuming as it is a simplified version of the others interaction models.

To verify if the interaction is being performed as expected we evaluate the quality of the performance tasks (successfully executed, successfully executed with mistakes, or not successfully executed) and the execution time spent on each of the 9 task. The balance between performance and the time spent to execute each task is crucial to the evalua-tion since there are no time limit defined. The tests were carried out considering 8 users (7 men and 1 woman, from 20 to 27 years old, students at the university or already graduated, with different levels of chemistry knowledge and where the majority had experienced Virtual Reality before) after signed an informed consent. To test the Model each user execute 9 tasks (**Error! Reference source not found.**) in a random order, with the exception of Task 9 the last one to be done since it allows to test all the previous features. The tests start with the users seat in front of a computer and place the HDM with the Leap Motion attached to it on their head and then the investigator started the Unity application.

After each task is completed, the investigator registered the time used to perform it, and if there were mistakes or incorrections during the execution. Due to the pandemic situation, all the tests were performed following sanitary rules. All the devices were protected with plastic film that was replaced between users. The hands of the users and of the investigator were washed with alcohol before and after the test. While performing the tests it was observed that sometimes users had troubles when performing the “thumbs-up” to indicate that the task was completed.

After the end of the test, the users report that they felt very confident using the system, evaluating it as simple and easy to use with no need for technical support and with few inconsistencies. Users also report some difficulties on the recognition of some hand figures to progress in or activate the modes of the game. This is a limitation of leap motion device here posibl associated with hand anatomy differences on the shape of fingers, for instance.

Performance metric assessed as percentage present 100% of success rate (with and without errors) for all developed modes with only the Rotation mode presenting a 92,9% rate.

The execution time of each tasks whithin each Mode was estimate calculating averages and standard deviations. Diferences higher than 30 seconds in average were defined as suggesting difficulties in task comprehension, reported for Translation and Link modes. Diferences higher than 30 seconds in standard deviations were defined as suggesting presenting possible incoherencies in execution, what was observed for Rotation Mode.

Usability evaluation shows that users would like to use this system frequently and found it easy to use. actually agreeing with the statement and finding it cumbersome to use.

It is important to note that for some users, the Leap Motion sensor failed to correctly capture their Hand Figure of “thumbs-up”, as mentioned

7. Conclusions

The present work exposes the development of an upgraded version of the interaction system of the game “Touch on Chemistry”.

New modes for the system were designed, each with a determined set of actions to be executed by the users, namely grab of objects, selection of groups of objects, translation and rotation of the groups, or linking of objects, organized in 9 different tasks. Furthermore, three interaction models were developed, each model focusing on different features that the Leap Motion has to offer. The One-Hand Detection Activation model was implement showing satisfying results in terms of interaction. The introduction of the concepts of Selection, Translation, Rotation, Link and Free Mode facilitated the process of cataloguing the actions.

With the system developed, it could be of value to see possible implementations in a different scope or area of knowledge, given that the base is a system for linking structures.

References

[1] “ACESSO AO ENSINO SUPERIOR 2020 RESULTADOS DA 1.ª FASE DO CONCURSO NACIONAL DE ACESSO,” *Direção Geral de Ensino Superior*, 2020. [Online]. Available: https://www.dges.gov.pt/coloc/2020/nota_cna20_1f_1.pdf.

[2] “Organic_chemistry Wikipedia.” .

[3] “Virtual: Search Online Etymology Dictionary,” *Index*. [Online]. Available: http://etymonline.com/search?q=virtual.

[4] C. Anthes, R. J. García-Hernández, M. Wiedemann, and D. Kranzlmüller, “State of the art of virtual reality technology,” *IEEE Aerosp. Conf. Proc.*, vol. 2016-June, no. March, 2016, doi: 10.1109/AERO.2016.7500674.

[5] M. Crespi, “The State of VR and AR,” *Qbit Technologies*. [Online]. Available: https://www.qbittech.com/index.php/vr-blog/item/136-the-state-of-vr-and-ar.

[6] K. Shimizu, “HOW TO: PREDICT THE TYPICAL NUMBER OF BONDS AND LONE PAIRS FOR EACH ATOM.” [Online]. Available: http://shimizu-uofsc.net/orgo/Chem_333/1a.ii.html.

[7] “Beat Saber,” *Beat Games*. [Online]. Available: http://beatsaber.com/.

[8] “Tetris Effect,” *Enhance*, 2019. [Online]. Available: https://www.tetriseffect.game/.

[9] T. S. Mujber, T. Szecsi, and M. S. J. Hashmi, “Virtual reality applications in manufacturing process simulation,” *J. Mater. Process. Technol.*, vol. 155–156, no. 1–3, pp. 1834–1838, 2004, doi: 10.1016/j.jmatprotec.2004.04.401.

[10] M. Virvou and G. Katsionis, “On the usability and likeability of virtual reality games for education: The case of VR-ENGAGE,” *Comput. Educ.*, vol. 50, no. 1, pp. 154–178, 2008, doi: 10.1016/j.compedu.2006.04.004.

[11] D. Barnard, “History of VR - Timeline of Events and Tech Development,”

VirtualSpeech, 2019. [Online]. Available: http://virtualspeech.com/blog/history-of-vr.

[12] R. McCartney, J. Yuan, and H. P. Bischof, “Gesture recognition with the leap motion controller,” *Proc. 2015 Int. Conf. Image Process. Comput. Vision, Pattern Recognition, IPCV 2015*, pp. 3–9, 2015.

[13] *2020, Laboratórios Abertos*, Maria Amél. Departamento de Engenharia Química, Instituto Superior Técnico.

,