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Touch on Chemistry - game to teach Organic Chemistry in Virtual Reality

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Abstract

The goal of this thesis is to create a game in Virtual Reality to teach Organic Chemistry.

Games are becoming more important in education, and as a result of that, more educational games are being created everyday in order to improve what traditional teaching methods lack. For this reason, the importance of educational games and methods used to create them, the good and bad aspects of the different games and applications already built and the possible solutions for the challenges inherent to VR applications and games were analysed.

The manipulation of objects is extremely important in Virtual Reality (VR) and it has other challenges that don't exist in a non Virtual Reality game. In this case, this aspect takes an central focus in the players will be interacting with atoms and molecules through out the game, and to make this manipulation as natural and easy to use as possible, the Leap Motion sensor was used in the project. The students will use their own hands to interact with the environment in the game and there are different methods that can be used according to the intended purpose.

The game consists on creating molecules by connecting atoms together to overcome the challenges presented and progress on the levels. The challenges are based on what high school students learn in their freshman year about Organic Chemistry, and the rules of how molecules are created must be followed. The implementation of the interaction with objects was achieve and all the game development was done in three iterations. Two tests were performed at the end of the first two iterations, one test per iteration, and a final test was performed at the of the last iteration with high school students and students from Instituto Superior Técnico.

The evaluation consisted on the users completing the tutorial and the Normal game mode, which was simplified and had four levels with two challenges each. The results were very positive, showing that the game is fun and entertaining, and that it has potential to be a helpful resource in a classroom.

Keywords

Virtual Reality; Organic Chemistry; Manipulation; Leap Motion; Game; Learning.

Resumo

O objectivo desta tese é criar um jogo para ensinar Química Orgânica em Realidade Virtual.

Os jogos estão a tornar-se cada vez mais importantes na educação, e por consequência há mais jogos educacionais a serem criados todos os dias para mitigar as falhas que alguns métodos tradicionais de ensino possuem. Por este motivo, foram analisados a importância dos jogos educacionais e os métodos utilizados para os criar, os aspectos positivos e negativos de vários jogos e aplicações que já existem e também as possíveis soluções para os desafios inerentes a aplicações de Realidade Virtual e jogos.

A manipulação de objectos é extremamente importante em Realidade Virtual e apresenta outros desafios que não existem em jogos que não usam tecnologia de Realidade Virtual. Neste caso, a interação com os objectos é um dos focos centrais deste jogo, pois os jogadores manipulam átomos e moléculas no decorrer do jogo inteiro, e para tornar esta interação o mais natural e fácil de utilizar possível, foi decidido utilizar o sensor Leap Motion neste projecto. Os alunos usam as próprias mãos para interagir com o jogo e existem diferentes métodos que podem ser utilizados, dependendo do objectivo da interação em questão.

O jogo consiste em criar moléculas, ligando os átomos uns aos outros, para ultrapassar os desafios que são apresentados e, por consequência, progredir nos níveis. Os desafios são baseados na matéria que é ensinada aos alunos do ensino secundário, especificamente no 10º ano, e as regras relacionadas com a junção dos átomos para criar as moléculas devem ser seguidas. A implementação da interação com objectos foi atingida e todo o desenvolvimento do jogo foi realizado em três iterações. Foram realizados dois testes no final das duas primeiras iterações, um testes para cada iteração, e houve também um teste final realizado com alunos do ensino secundário e com alunos do Instituto Superior Técnico, no final da última iteração.

A avalição consistiam em completar o tutorial e o modo de jogo Normal, que foi simplificado, tendo apenas quatro níveis com dois desafios em cada um. Os resultados foram bastante positivos, pois

mostram que o jogo é divertido e agradável, e que tem potencial para ser usado numa aula.

Palavras Chave

Realidade Virtual;Química Orgânica;Manipulação; Leap Motion; Jogo; Aprendizagem.

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Introduction

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1.1 Motivation

Nowadays, there are more and more educational games being made that can have impact and meaningfulness in several fields of studies. There are a lot of studies that expose the positive results that games have in education, for different subjects such as mathematics and science, making the learning experience more fun to the learner. Some of these studies were analyzed and depicted in this document.

However, this is not an easy task since there is no flawless guideline to create a good educational game. There are many problems when trying to integrate games in education, the most common one is that the focus is mainly on the teaching aspect and the fun and engaging part is left out. This takes out the motivation in playing the game, thus making the learner not willing to play it. There has to be a balance between both aspects, teaching and entertainment, in order to have a game that has greater chances to achieve its goals.

Not only is gaming becoming more important in education, Virtual Reality is also being taken into account since it provides a platform where learners can be fully immersed in a virtual world allowing them to perform actions that they couldn't do in real life. It also has a major impact in helping students understand abstract concepts in a more concrete way. Besides that, both VR and games allow the players to solve problems that could be dangerous in real life without having to be concerned about being in a possible hazardous situation.

This project aims to improve and complement the traditional methods of teaching Organic Chemistry. The most prevalent issue in these traditional methods is the way that molecular structures are presented to students which is based on the ball-stick model. Most organic compounds structures are easily understood through this model, however it gets tricky when they get more complex. With Virtual Reality, it is possible to create a game that adds interactivity and immersion to these traditional methods, thus enabling the students to understand better the more difficult subjects.

With the Virtual Reality technology, comes the challenge of how the interaction with objects should be performed. To help with this aspect, this project also makes use of the Leap Motion which tracks the user's hands, enabling the use of the hands to perform the manipulations in the virtual world, instead of using hand held controllers.

1.2 Objectives

The main objective of this thesis is to develop an Organic Chemistry game using Virtual Reality technology for high school students in order to add more interactivity in the learning process of the subject. Also the levels and challenges of the game can be changed by the professors to fit their objectives for each class. This game is a complement to the classes and it doesn't substitute the learning

process of the class, it is an extension to the existing learning methods. This means that the players that experiment this game should have some previous knowledge about the domain, because it doesn't teach everything from the beginning.

To achieve the main goal, another important topic needs be covered in this thesis, which is how the manipulation of objects can be made within a virtual world with our own hands. This is a vital aspect because the game is focused on the interaction with atoms and molecules, making it relevant to thoroughly analyze different ways to have these manipulations in Virtual Reality.

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Background

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2.1 Domain

2.1.1 Organic Chemistry

Organic Chemistry is a chemistry subdiscipline that focuses on the study of the structure, properties, composition and reactions of organic compounds and organic materials. The range of chemicals studied include hydrocarbons which are carbon-containing compounds and also many other compositions that are always based on carbon and hydrogen but with other elements like oxygen, nitrogen, sulfur, phosphorus and halogens.

The study of the structure of these organic compounds includes several physical and chemical methods that are used to determine their chemical composition and chemical properties. Regarding the properties, which incorporates both physical and chemical properties, the same methods used for the structure study are applied, and also some methods to evaluate chemical reactivity. Lastly, the study of reactions mostly tests their scope through use in preparation of target compounds by chemical synthesis.

Organic chemistry used to be limited to compounds produced by living organisms but nowadays includes human-made substances such as plastics, fuels and explosives, pharmaceuticals, among others. Everyday organic chemists spend much of their time creating new compounds and developing better ways of synthesizing already known compounds.

2.1.1.1 Nomenclature

The names of organic compounds can be either systematic or nonsystematic. The first type follows logically from a set of rules that are stipulated by the International Union of Pure and Applied Chemistry, commonly referred as IUPAC. Since it is a rational nomenclature system it should be able to provide two major features: it should indicate how the carbon atoms of a given compound are bonded together in a characteristic structure of chains and rings, and it should identify and locate any functional groups present in the compound. An IUPAC name will have three essential aspects: (1) a root or base indicating a major chain or ring of carbon atoms found in the molecular structure;(2) a suffix or other element(s) designating functional groups that may be present in the compound;(3) names of substituent groups, other than hydrogen, that complete the molecular structure.
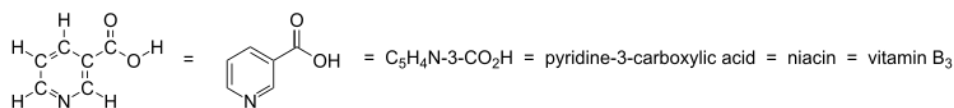
Figure 2.1: Example of a nomenclature.

This system avoids problems caused by arbitrary nomenclature due to its set of logical rules because together with a structural formula, one should be able to write an unique name for every different com-

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pound. However, it is burdensome to use this set of rules for complex molecules, so they are usually more rigorously followed for simple compounds.

The nonsystematic nomenclature is simpler but only unambiguous to organic chemists, since their names do not indicate the structure of the compound. They are more commonly used for complex molecules, which encompass most natural products.

2.1.1.2 Structural drawings

A structural formula shows how the various atoms are bonded to each other, and this can be done in 2D or 3D. In the 2D version there is the displayed formula where each endpoint or intersection is an atom and all the bonds in the molecule are shown as individual lines. The fact that carbon has four bonds, nitrogen three, oxygen two and hydrogen one, makes the representation of these molecules greatly simplified. Besides that, one molecule doesn´t have a specific order or place to draw each atoms, the only rule that one must respect is the number of bonds and to which atoms each atom is linked to.

Figure 2.2: Structure of organic compound with different representations.

There is also the line-angle formula, also called skeletal formula, which is simple and unambiguous. In this formula, the endpoints and intersections of each line represent one carbon and the hydrogen atoms are removed from carbon chains. This means that they are represented along side each carbon atom, and there have to be enough hydrogen atoms attached to each those carbon atoms to make the total number of bonds up to 4. This way it is just left a carbon skeleton with functional groups attached to it. The line-angle formula is particularly useful to represent rings of carbon atoms, which can be difficult to draw tidily in a normal structural formula.
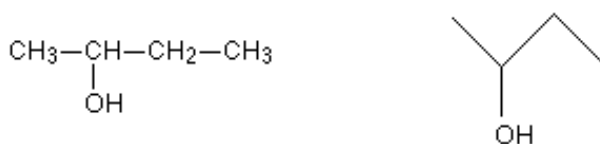
Figure 2.3: Example of skeletal formula

The 3D version might be useful in some occasions and the symbols change a bit to represent different positions of the atoms in 3D space on paper:
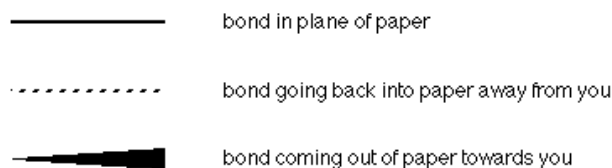
Figure 2.4: Symbols to draw 3D structure.

With this type of structural drawing it is easier to show rotations of the bonds between the atoms.

2.1.1.3 Bonds

A molecule consists on a group of atoms bonded together. The way the connect with each other is directly related to their valence electrons, which are outer shell electrons that are associated with an atom, and that can participate in the formation of a chemical bond if the outer shell is not closed. For example, in a single covalent bond, both atoms in the bond contribute one valence electron in order to form a shared pair. The presence of valence electrons can determine the element's chemical properties, such as its valence — whether it may bond with other elements and, if so, with how many.

Atoms will react to get in the most stable state possible. A complete octet is very stable because all orbitals will be full, which means all elements want to have a full outer shell (eight electrons), and when they don't have enough valence electrons by themselves to fill the outer shell, they can form a covalent bond with other atoms by sharing their valence electrons. An example of this is when two oxygen atoms (six valence electrons) encounter carbon (four valence electrons). Because each atom wants to have eight electrons in its outer shell, the carbon atom shares two of its valence electrons with each oxygen atom, completing their shells, while each oxygen atom shares two electrons with the carbon atom to complete its shell. The figure 2.5 depicts how many valence electrons the most relevant types of atoms in Organic Chemistry have, and how many bonds they can have.

Atom type	Carbon	Hydrogen	Oxygen	Bromine	Fluorine	Chlorine	Iodine
Valence electrons	4	1	2	7	7	7	7
Number of bonds	4	1	2	1	1	1	1

Figure 2.5: Types of atoms with their valence electrons

There are some exceptions to the octet rule which are: when there are an odd number of valence electrons, when there are too few valence electrons and when there are too many valence electrons. The main exception to the rule is hydrogen, which is at its lowest energy when it has two electrons in its valence shell, which means he only needs to make one bond to become stable.

2.1.1.4 Functional groups

Functional groups are specific groups of atoms within molecules that have very characteristic properties regardless of the other atoms present in a molecule – alcohols, amines, carboxylic acids, ketones, and ethers are all common examples. The main characteristic that they possess is that they have specific bonding arrangements between specific atoms. For example, for a molecule to be considered an alcohol, a carbon is single-bonded to an OH group (the OH group consists of an Oxygen atom bonded to a Hydrogen atom).

The figure 2.6 displays some of the most common functional groups.
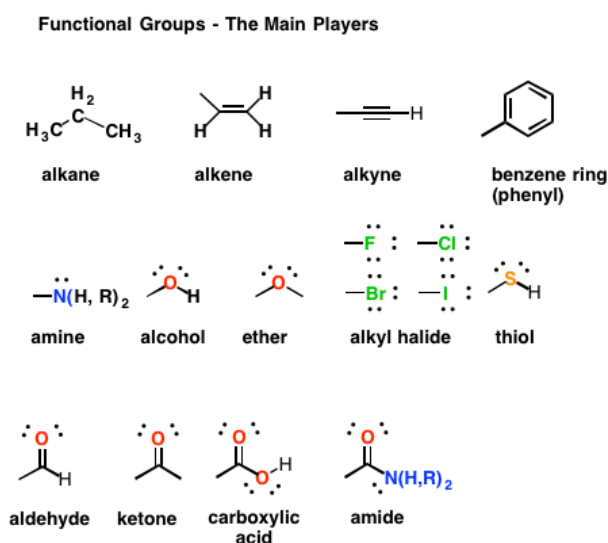
Figure 2.6: Functional groups

2.1.2 Discipline topics

Organic Chemistry is a field of study that has several components that are taught to students of several levels of education, but for this game, the focus will be on the subjects that are taught to high school students.

From research made to find out what high school students learn about Organic Chemistry[1] [2], the following learning objectives were defined:

- Bonding and structure of the molecules

- Fundamental groups (alkane, alkene, alkyne, benzene ring, amine, alcohol, ether, alkyl halide, thiol, aldehyde, ketone, ester, carboxylic acide and amide) and homologous series

- Systematic nomenclature

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[1] http://www.stc.edu.hk/home/life/curriculum/chem.pdf [accessed: 20/12/2017]
[2] http://pubs.acs.org/doi/abs/10.1021/ed024p244?journalCode=jceda8 [accessed: 20/12/2017]

- Isomerism

- Organic acids and organic bases

- Reaction mechanism

These are the overall goals in Organic Chemistry courses, however they will not all be learning objectives in the game that will be developed. This will be further explained in the Implementation section.

2.2 Games and Education

Games are becoming a sought out tool to enhance the teaching of several disciplines, ranging from high school to college subjects. There are studies that show that games have a positive impact in changes in perception, attention and spatial cognition [2]. Low-level sensory processes and higher-level cognitive processes are interrelated, and although those low-level processes are insusceptible to the effects of training, there have been some studies that demonstrated an improvement in visual spatial resolution after training with an action video game. There also many experiments in psychology that show that many of the higher-level processes can be modified through training, making it possible to assume that playing videos games can have impact in basic attentional processes because they are influenced by higher-level cognitive processing [2].

Although this study [2] focuses on the impact of FPS videos games, there are some general conclusions drawn from it that can be applied to any educational games, mainly the workflow for game design presented. There are six steps in it: (1) determine the purpose and psychological domain of the game; (2) list the cognitive processes that are relevant; (3) list the game attributes and requirements; (4) select a game theme to integrate all attributes; (5) be aware of individual differences in cognitive abilities in the target groups and create a range of entries with different difficulty levels appropriate to these individual differences; (6) test the effectiveness of the game by measuring cognitive performance of individuals from the population of interest before and after playing the game. This workflow can also be applied to games that aim to help those with some kind of health or mental issue, for example, Alzheimer's and ADHD, where the goal is to improve certain cognitive processes, and through this guideline, one can structure how the game should be made.

From these results, we can assume that games can have an impact in teaching, but creating an useful and fun educational game is not an easy task. There has to be a balance between the educational purpose and the entertainment aspect for the game to improve learning and be engaging at the same time. There have been some studies that create a connection between educational theory and game design so that the games created are meaningful and engaging. Kiili [3] distinguishes three major components to design educational games: the person, the task and the artifact, which is a term that

covers tools and toys. He claims that the aim of an educational game is to provide challenges related to the main task, making the flow experience possible, and in order to so, the artifacts can't be complex thus allowing the player to focus on higher order tasks.

He proposes a model that links gameplay with experiential learning to facilitate flow experience, and describes the learning process as a cyclic process through direct experience in the game world. The base of this model are the challenges based on educational objectives provided in the game. First with clear goals, also provided by the game, taking into consideration the resources available in the game world, and using it's creativity, the user can draw conclusions and form hypotheses, leading to active experimentation, after which the game gives feedback allowing the player to observe and reflect on the results. The cycle then repeats itself and ultimately leads to the discovery of new and better solutions for the challenge being tackled.

However, not only is important to keep in mind the relationship between game play and educational objectives, one mustn't forget the believability aspect in the game. This component is more relevant than authenticity, meaning that content presentation must be believable within the context of the game [4]. All the puzzles, problems and challenges should appear logically from the narrative structure of the game and need to be challenging enough to incite players to broaden out their knowledge and assimilate into their existing schemata through discovery, trial and error strategies. Royle also says that the existence of cheats is relevant in an educational game, because the moment a player searches for extra knowledge an independent learning strategy is invoked. For this reason, the search for cheats is pedagogically important.

2.3 Chemistry Games

Scientific fiels such as chemistry are usually described as a hard to learn subjects due to its amount of abstract concepts. Because of this, games are being introduced in the classroom in order to stimulate students to learn in a more enjoyable way.

Most chemistry games, that exist to date, are more commonly card games or boardgames whose objectives are to help students memorize the periodic table, distinguish the several elements by knowing their names, atomic number, symbols and properties, and also connect the different molecular structures with their names. Go Chemistry is an example of that, it is a game that is similar to Go Fish and the objective is to correctly form the formulas of covalent and ionic compounds and then providing their names [5]. Groupica, Compoundica and Elemental Periodica are a set of three games that encompass many interralated subjects and concepts of chemistry [6]. Groupica is similar to the card game "The Families of Chemical Elements", and the goal is to collect complete sets of cards depicting group families of the elements. Elemental Periodica is a Bingo style game where students are given a card with the

periodic table drawn on it along with the elements they need to collect. A referee will be reading the cards that contain the elements, but he will only read information about it, which is its atomic number, block and properties related to daily life or technology, without saying its name or symbol. The players must guess which element the referee is talking about and if they have it on their periodic table, they should mark it. This way the students are stimulated to connect the concept of the elements to both the periodic table and to daily life. Compoundica is a board game where the players must form compounds.
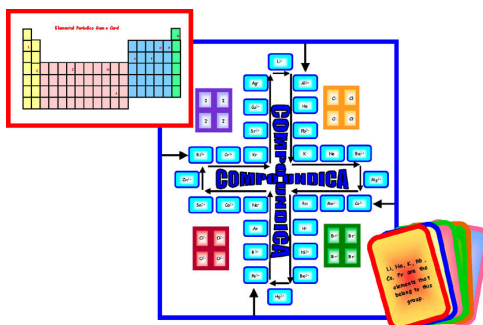
Figure 2.7: Compoundica [13]

These games are some examples of what has been done regarding games in chemistry, and the results obtained from their testing were very positive. In this study [6] both students and teachers said that it was an interesting and enjoyable way to learn chemistry concepts, and the students retained their knowledge better than being taught through a traditional method. Rastegarpour and Marashi [7] stated that card games and computer games methods of teaching are effective tools for learning chemistry concepts. Their study with a controlled pretest and posttest design to analyze the effect of these two methods showed that there is a significant difference between the posttest scores for learning through computer and card games and the traditional method.

2.3.1 Organic Chemistry Games

Just like general chemistry games, most organic chemistry games are a card game or a board game, however they mainly focus on the nomenclature and structure connection of molecular compounds. Zanon, Guerreiro & Oliveira [8] created a didactic game for students to learn the nomenclature of organic compounds and it was designed to stimulate cooperativeness. It is a board game meant to be played in teams thus promoting cooperation between the players. There are 100 cards with questions, 20 challenge cards and 20 joker cards, and each time a team has to draw one of those cards depending on the position they are in the board. The question cards can have the nomenclature of the molecule and the players need to draw the structure, or the opposite as well. The results from its application were positive, the students were able to expand their knowledge on the nomenclature of different compounds and also to identify the bondings in each molecule. It also had showed that students like to play cooperatively,

Figure 2.8: React! Chemistry game

since 85% stated in a post questionnaire that they prefer to play against teams, rather than one on one.

A group of undergrads at UC Berkeley created a board game called React! (figure 2.8) which is a multi player game that aims to help anyone learn college-level organic chemistry. The basis of the game is to buy and trade chemicals, discover and perform reactions, and create special molecules. In order to discover and perform reactions, the players have to draw and transform chemical functional groups to create new molecules, thus allowing them to practice organic chemistry concepts. Besides that it has simple rules that are easily understood, and most of the feedback from the hundreds of students varying from high school to college, was very positive, stating that it was a fun and interesting way to learn organic chemistry and it brought excitement in learning this discipline.

2.3.2 Organic Chemistry Applications

Besides the several card and board games about organic chemistry, there are also applications and tools that are useful in this field and are being increasingly developed nowadays. Most of them have either Augmented Reality or Virtual Reality technology, since in this discipline the focus is restrained on relating the different molecular structures to their nomenclature and also on the bonding of the molecules. Because of the physical aspect of these concepts, those technologies are the best choice to create a application, since they enable the users to have a more concrete visualization and direct interaction with the subject, rather than using the traditional methods, like the ball-stick model and Van der Walls spherical model that have some issues. Although these models provide a good understanding of the structural and spatial relationship of molecules, they fail to give a grasp of the forces present in the interactions between the atoms involved in atomic bonding. For this reason, AR and VR applications are being used to fill the gaps left by these traditional methods.

One example using Augmented Reality technology is Augmented Chemistry [1] which is an application based on a Tangible User Interface. It allows the users to interact with 3D molecules in a intuitive
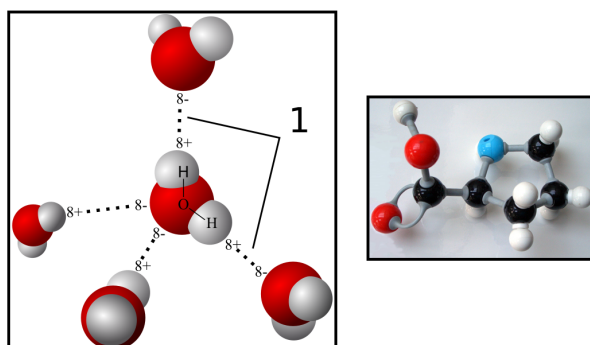
Figure 2.9: Ball-stick model

and direct way, and it enables them to build molecular models. The interaction in this system is made through a booklet, a platform, a cube and a so-called Gripper. The Gripper is a tool that allows users to pick an element and binding it to a molecule, while the cube enables the rotation of the molecule. The platform holds the molecule and the booklet shows all the elements that the user can pick. As for feedback, since there is no tactile method to tell the user what is happening, audio was used as a substitute. Whenever a molecule has no more bindings left or when it belongs to a predefined list, there is a sound that is played accordingly. Although this is not a game, it approaches and implements the mechanisms that are fundamental in the interaction with atoms and molecules, particularly the feedback aspect, which is crucial in the game to be made.

Figure 2.10: The Gripper tool [1]

There are, however, some applications that use haptic enhancements as feedback, which is a bit closer to a real life experience because it recreates the sense of touch by applying forces, vibrations or motions to the user. This type of feedback is particularly used for demonstrating the forces involved in the bonding process of a molecule. There is a computer-modeling program in which the user can feel the electrostatic forces between atoms and groups of atoms, while building the different molecules [9]. This system uses a keyboard and the PHANTOM haptic interface, which is a device for probing virtual objects. This device measures the user's finger tip position and exerts a precisely controlled force vector on it. The atoms can be in four different states: unplaced, held, fixed or bonded, and they represented the stages of bonding an atom to a molecule. In each iteration, the forces between every atom that is either held, fixed or bonded are calculated and is given haptic feedback to the user according to those

forces. A similar system uses augmented reality, voice commands and haptic feedback to provide the same sense of forces in the bonding process of molecules [10]. This is a multi-modality interface used for observing complex molecular structures that provides an intuitive way of understanding the underlying working principle of this subject.

Another good way to have an application with tactile feedback is the use of some sort of glove that can provide these type of responses. The Data Glove is an example of that, it was created by Prachi D. and D.R. Patil, using Contact Lever Switch, and it was used for a tool that allows the users to manipulate the molecules, but they cannot build them at runtime.

Another example of this types of application is MolyPoly, a 3D immersive gesture controlled approach to visuo-spacial learning of organic chemistry [11]. This system uses a different method to interact with the molecules based on gestures and using a manipulation panel to aid on the interaction. The gestures are detected with the Kinect skeletal tracking, which detects the position of both hands and they are represented in the 3D environment. The manipulation panel has the options of rotate, zoom, provide feedback and delete an atom. The feedback mentioned are explanations about the molecules in audio format. Just like in Augmented Chemistry, there is no tactile mechanism being used, so the feedback for this application rests on audio. Every time a user builds a molecule he receives some audio response to let them know if they build it correctly or not, besides giving them explanations about the molecule. To test the effectiveness of this tool in learning organic chemistry, a group of 17 students was divided into 2 groups, where one was taught with the traditional methods, and the other one used MolyPoly. All of them took a pre test and a post test, and in the post test it was revealed that there was a statistical significant improvement for the low and high spatial knowledge questions for the group that used MolyPoly, although there was no significance when there is no spatial knowledge involved.

2.3.3   Games and applications review

The majority of games, that exist to date, about Chemistry and Organic Chemistry are board games or card games. Some of them are variations of well-known games like Bingo and Go Fish, making them faster to learn and easier to play. Other games are built from scratch without an existent game as a base, like the didactic game created by Zanon, Guerreiro & Oliveira..

These games aim to improve the students knowledge of different subjects in the disciplines, with emphasis on memorizing the periodic table, distinguish several elements by knowing information about them, connect molecular structures to their nomenclatures and identify the bondings in the molecules. Some of them also encourage cooperation because they are design to be played as team.

Even though there aren't many Organic Chemistry games that aren't a board or cards game, they still provide results and mechanics that can be applied or adapted into the game that will be made through this project. Some of them are the mechanics of correlating names and nomenclatures to

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the molecules, identifying their bondings and knowing the different elements. The use of the games showed improvement in retaining knowledge and were categorized as a fun and interesting way to learn chemistry concepts.

From the applications that were analyzed it is possible to obtain good insights about how to create the interaction with the molecules. The Augmented Chemistry depicts the manipulation of atoms and molecules through different tools using augmented reality. The same concepts of manipulation can be applied to the game to be made, specifically picking atoms, connecting them to create a molecule and rotate the molecule built. This particular application also provides non haptic feedback, which is also the case with the game that will be created, instead it as audio feedback, making it a good example as to how to use other types of feedback.

The MolyPoly application also provides useful information regarding feedback and manipulation of molecules. Not only does it have a similar implementation of audio feedback as the Augmented Chemistry, but it also provides explanations about the molecules in audio format as well. This component can be used in the game to be created, in order to help students learn more about the organic chemistry concepts. Regarding the manipulation of atoms it implements mechanisms of zoom, rotation and delete, which can also be applied in the game that is going to be made.

Overall, the games and applications depicted in this document have useful information that can be used in the game that is going to be created. But it lacks content about visual feedback, which combined with audio feedback can produce results almost as good as a system that has haptic feedback. This is a component that will be explored.

Another aspect that should be considered is the naturalness of the interactions with the molecules. MolyPoly displays a menu that shows the different type of interaction available to the user, and by selecting them he can then perform the intended manipulation. This is a functional and easy to use solution, but it can be improved by removing the menu and creating natural and easy to learn gestures that perform each interaction. This is a component that will be implemented and tested to figure out which method works the best.

2.4   Virtual Reality in Education

According to the constructivist theory by Piaget humans construct knowledge by learning from their experiences[3]. This makes the learning process a form of active hypothesis testing rather than a passive accumulation of acceptance of facts, which is the most common way of teaching nowadays, using methods such as lectures and demonstrations in the classroom[4]. This theory implies that a person learns in real life by doing and improves his skills through practice on realistic tasks, meaning that there must

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[3]https://en.wikipedia.org/wiki/Constructivism_(philosophy_of_education) [accessed 3/1/2018]
[4] https://en.wikipedia.org/wiki/Teaching_method [accessed 3/1/2018]

be active learning in order to have improvement. Since humans learn by having experiences and by interacting with their environment and using their senses to derive information from the world, Virtual Reality becomes a clear choice to create educational games.

Virtual Reality is broadly applicable to the many areas in education due to the myriad of scenarios it can be used to explore. A major feature of VR is that it allows multi-sensory interaction with the space visualized, making it possible to experience subjects that would be difficult or even impossible to illustrate with the traditional teaching methods. Not only that, but it takes out any dangerous situation or difficulty that a student would normally encounter in real life. When creating a VR game or tool, there are three aspects to consider: immersion, interactivity and multi-sensory feedback [12]. Being immersed means being enveloped or surrounded by the environment, and the key benefit of immersion is that ensures a presence or the feeling that one is really in the virtual world [12]. Interactivity is the ability to control events in the virtual world using one's body movements and having the world generate responses to them. Last but not least, multi-sensory nature allows the simulation to be more believable and engaging because the information is derived from several senses making it more redundant which reduces potential ambiguity and confusion. These features make VR a great option to use in educational games, because it means that a student can be put in a depicted world, experiment and interact with it, generating solutions to problems that are thrown at him, and having responses from the world to those actions, within a safe environment.

Keeping in mind the constructivist theory and the three key features of VR, there are 5 strategies to design Virtual Reality Learning Environments [13] that one can use. They are situated learning, role playing, cooperative and collaborative learning, problem based learning and creative learning. This paper will focus on problem based learning which is a learner-centered approach that encourages learners to solve a problem by outlining a problem. The goal for this strategy is to fill the gaps that a strictly passive teaching method has by encouraging learners to develop independent thinking ability and collaborative learning. It allows students to observe the simulated situation, motivate them to learn and solve problems adequately through the immersive interactive environment [13].

2.5   Objects manipulation in Virtual Reality

The interaction with objects within the virtual world is an important issue to tackle, because if this component is not functioning properly, it will negatively affect the immersive feeling of the virtual environment, thus impacting the whole experience. In the game to be developed in specific, the interaction with objects (atoms and molecules) is extremely important, thus it is necessary to understand how to manipulate objects in a virtual world.

There are a couple of aspects that need to be explored for this component to be implemented: the

technique or techniques used and also the device.

2.5.1 Taxonomy

A taxonomy has been created by Poupyrev and Ichikawa (figure 2.11) that categorizes the different methods of virtual objects manipulation available at the time by analyzing their characteristics and see their similarities [14].

Poupyrev and Ichikawa categorized the techniques according to their basic interaction metaphors into exocentric and egocentric techniques. An exocentric method use what is known as the God's eye viewpoint, meaning that the users interact with the virtual world from the outside. Some examples of this type of techniques are the World In Miniature and World Scaling, which will be detailed further in the section. On the other hand, in an egocentric technique, which is the most common type, the user interacts with the virtual environment from the inside. In this category we find the virtual hands and the virtual pointers.
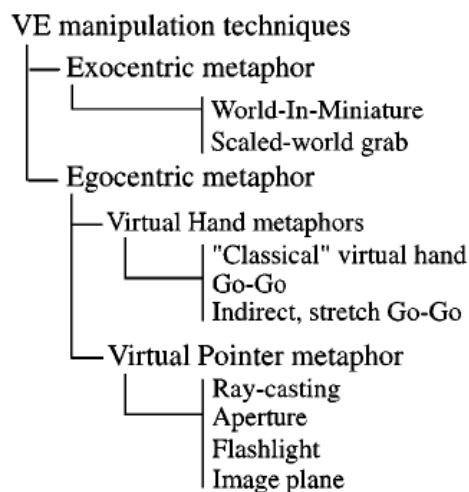
Figure 2.11: Taxonomy proposed by Poupyrev and Ichikawa.

A – Manipulation techniques

There are several techniques that can be used for manipulating objects, each having its advantages and disadvantages, but one aspect that they all must have is that they should provide the means to accomplish at least one of the three basic manipulation tasks: object selection, object positioning and object orientation.

Early methods attempted to directly simulate real world manipulation, creating a natural interaction with the virtual environment and requiring less effort from the users to use it. However, these techniques have some constraints that recent techniques can overcome, allowing the users to manipulate the virtual

objects in new ways which are not possible in the real world. Although there are many techniques used for manipulation of objects, there are two major categories: virtual hands and virtual pointers. The classical virtual hand one provides direct manipulation capabilities by resembling the user's real hand in a virtual space. This method is intuitive and natural due to the direct control of objects based on analogies from the real world, but the user is restricted to the physical reachable area around him. The virtual pointer can expand the reachable area by allowing the user to cast a ray at a distant object that enables the user to pick it, grab it and interact with it. Because of the ray cast, this technique requires relatively less effort to perform any manipulation to the object. This is due to the depth that the object is regarding the user, since moving an object that is farther away requires less physical movement than moving an object that is closer, considering that the distance moved for both of them is the same. Although this is considered a easier technique to use and also more efficient, it can be subjected to inaccuracy due to hand jitter and the Heisenberg effect.
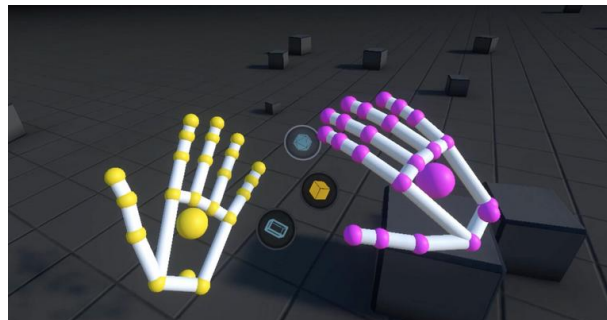
Figure 2.12: Example of a classical virtual hand

Hand jitter is hand tremor that naturally occurs to any person, and is particularly noticeable in free-hand 3D input devices, which are commonly used in VR applications and games. This causes some difficulty in accurately point and select an object, specially if the object is in a farther distance. The Heisenberg effect[5] is defined as the uncertainty principle states that (in particle physics experiments) the very act of observing alters the position of the particle being observed, and makes it impossible (even in theory) to accurately predict its behavior. In the case of virtual pointers, it is related to the uncertainty between pointing and selection gesture.

In order to overcome the obstacles related to the classical virtual hand, there are other techniques that have been created that aren't virtual pointers. One example is the Go-Go technique, which uses the metaphor of interactively growing the user's arm and non-linear mapping for reaching and manipulating distant objects [15]. In this technique, there are two areas defined, one that uses linear mapping and another one that uses non-linear mapping. When the user's hand is within a local area defined between the position of the user and a certain distance (it is two thirds of the user's arm length), he manipulates the objects with an 1-to-1 ratio. This means that the movement of the virtual hand matches the movement

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[5]http://www.businessdictionary.com/definition/Heisenberg-effect.html [accessed: 28/12/2017]

of the real hand. When the user's hand is further than the set distance, the mapping is non-linear and the virtual arm grows. Because this technique maintains the same metaphor as the classical virtual hands technique, it makes it highly intuitive and easy to use.

Even though the Go-Go techniques solves some issues related to the classical virtual hand, it still presents some of its own difficulties, the main one being that it has finite range. Thus some variations of the Go-Go method were made in order to fill the gaps in the original technique. The variations created were the Stretch Go-Go, the Indirect Stretching and the Fast Go-Go techniques [16]. The first one uses 3 different discrete velocities in 3 different concentric regions defined around the user. The virtual hand is in the middle region, and it grows at a constant speed when it is in the outermost region, and it retracts a that same speed when it is in the innermost region. The Indirect Stretching works just like the Stretch Go-Go but the growth and retraction of the virtual is made through buttons on a 3D mouse. Although it may be more precise and physically easy to use, this has the disadvantage of taking away the natural metaphor, which is one of the strongest points that characterizes this type of methods. Finally, the Fast Go-Go maps the physical hand velocity to the rate of growth of the virtual arm, and it can be added to the indirect stretching technique.

Poupyrev and Ichikawa also tested some of these techniques for different basic types of virtual object manipulation in order to verify which one was better. The techniques tested were the Go-Go, ray-casting and classical virtual hand. Regarding selection tasks, for both the virtual hand and the virtual pointer their comparable weaknesses and strengths depend on the particular conditions of the task, for example, with increased distance and high accuracy, the ray-casting techniques rapidly degraded their performance. In positioning tasks, all techniques show the same performance within the area of reach, however for greater distance the ray-casting requires less movement than the Go-Go to reposition an object. Without change of distance or with constant speed, the classical virtual hand and the ray-casting outperformed the Go-Go technique. From this results, we can conclude that there isn't a 'better' technique to use for each type of basic manipulation since their performances can only be compared in relation to the particular conditions of the spatial manipulation.

Because these two types of techniques have different performances for different types of object manipulation, there have been some hybrid techniques that try to use the best characteristics of both types. One of them is the HOMER technique [16]. This hybrid method was created considering the results of an informal usability study concerning the manipulation of virtual objects using 6 techniques: Go-Go, Stretch Go-Go, Indirect Stretching, Fast Go-Go, Ray-casting and Reel ray-casting. The manipulation tasks included grabbing, manipulating and releasing the object. From this study they concluded that none of the techniques were easy to use and efficient enough throughout the entire interaction that includes those manipulation tasks. Their biggest finding was that grabbing and manipulating an object must be considered separately for overall usability, since it was easier to grab an object with ray-casting,

but arm-extension techniques were preferred for object manipulation. Thus the HOMER technique uses ray-casting for object grabbing and hand-centered manipulation, using the best of both types of techniques. The user grabs the object with a light ray and then a virtual hand moves to the object position and it is attached to the hand. From this point, the user can manipulate the object using the virtual hand, and once he releases the object, the hand returns to its original position. The main advantages of this technique are that object grabbing is easier and object distance is also easier to control and the manipulation requires less physical effort.

There are other techniques that can be used to manipulate virtual objects which fall in the category of exocentric viewpoint, meaning that they control the objects from outside the scene. Some examples of this type of techniques are the World in Miniature and Voodoo Dolls. In the WIM method the user has a replica of the scene in his hand, including all of the objects and the a representation of himself in the scene. He can pick up objects from the replica with the other hand and reposition them anywhere within the world in miniature. However it has some issues, one of them being not providing sufficient accuracy, because with a large ratio, small motions in the WIM result in large motions in the 'real world', making accurate placement difficult. The Voodoo Dolls technique overcomes this problem by using a hand-held representation of a small section of the world centered on a particular object [17]. The user specifies the center of the context by image plane selecting an object, creating a doll (a transient, hand held copy of the selected object), which he can then manipulate. This technique works for a broad range of object sizes, allows users to manipulate both nearby and distant objects and allows users to accurately position objects when the target position is nearby or far away.

While the classical hand is very useful for manipulation with objects closer to the user, the virtual pointer is better to interact with objects that are farther away from the user. It is also particularly good with interactions with some interfaces, like menus. For this project, the classical hand will be mostly used for the manipulation of objects, since they will be close to the players. However, the virtual pointer might be used for any menu that may be implemented, which means that there must be a clear distinction between situations where the player is using a classical hand or when he is using a virtual pointer, to make sure that he isn't confused about which one he is using at any point of the game.

2.5.2 Feedback

One important aspect regarding the manipulation of objects in Virtual Reality is the feedback that is given to the player when he performs different actions in the virtual world. The best type of feedback that can be used in a VR game or application is haptic feedback, which allows the user to have the sensation of touching a virtual object by simulating some features of the object such as: hardness, weight, inertia, surface contact geometry, smoothness and slippage. However, the hardware that was available to use in this project didn't have haptic feedback, making it necessary to find an alternative whose results should

be as close as possible to the results of using haptic feedback.

Most games and applications rely on visual and auditory feedback which, comparing to haptic feedback, are a low-cost type of feedback. The visual and auditory sensorial channels have a one-way, information-only flow, which means that they only collect and analyse information coming from the environment but have no interaction with it. Also, these two senses are allocated to relatively large areas in the sensory cortex, suggesting that visual and auditory displays have the potential of presenting haptic feedback with good results [18]. For this reason, the chosen replacement for haptic feedback was the combination of auditory and visual feedback.

2.5.3 Hardware

There are several hardware options that can be used for manipulating objects. The main factors that influence the choice are the feedback that we can retrieve from them, their ease of use, accuracy and area of reach.

2.5.3.1 Gloves

To this date, there are many gloves built for interaction purposes in virtual environments that allow the users to have a bigger immersive feeling in a virtual world, and also enhances the use of real world analogies to manipulate objects within the virtual environment. Besides that, most of them also provide haptic feedback which is a huge plus when it comes to manipulating virtual objects. Haptic feedback includes three types of feedback: force, tactile and proprioceptive. The force feedback allows the users to get the sensation of touching a virtual object, and gives an even greater immersive feeling within the VE since it simulates object hardness, weight and inertia. Tactile feedback simulates surface contact geometry, smoothness, slippage and temperature, while proprioceptive feedback gives a sense of the user's body position or posture [19].

There are some studies that verify the effect of force feedback on virtual object manipulation compared with visual and auditory feedback. One of these studies' conclusions [18] showed that haptic feedback alone has better results than the other two types of feedback, but the combination of haptic and audio responses was the one with the smallest error rates. This means that, although the users can have a great immersive virtual experience with haptic feedback alone, it is not the option that provides the best results.

Some examples of this type of hardware are VRgluv[6], Manus VR[7], Dexmo[8], VRFree[9], and many more. Most of these gloves are compatible with several virtual reality systems and provide some kind of

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[6]https://www.vrgluv.com/ [accessed: 13/12/2017]
[7]https://manus-vr.com/ [accessed: 13/12/2017]
[8]http://www.dextarobotics.com/ [accessed: 13/12/2017]
[9]http://www.sensoryx.com/ [accessed: 13/12/2017]

haptic feedback, making them great options for virtual interaction.
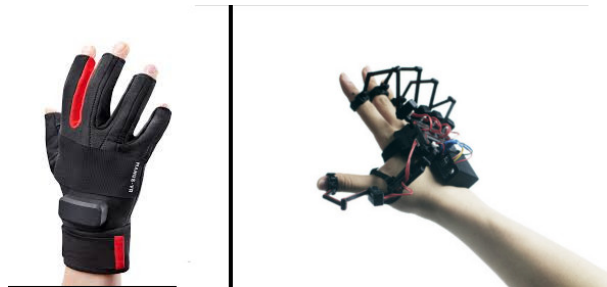
Figure 2.13: ManusVR on the left and Dexmo on the right.

2.5.3.2 Hand-held controller

Another commonly used hardware on virtual systems are hand-held controllers that are used to simulate the user's hand within the virtual world. Although this is usually the hardware that requires less effort from user to interact with the virtual environment, it is the less natural and it barely follows the real world analogies of object manipulation. Hand-held controllers rely mostly on buttons and track pads to perform the majority of the tasks associated with interaction within a virtual world. But they also have sensors that track their position, allowing the use of arm motions in the VE, which means they provide a bit of a natural interaction in certain tasks.

Most hand-held controllers are built specifically for a certain virtual system, like the HTC Vive or the PlayStation VR.

Figure 2.14: HTC Vive controller

2.5.3.3 Full body sensor

Full body sensors allow a full immersion in the virtual world by tracking the user's whole body and it provides them the ability to feel control over their full virtual body.

There are already some systems developed that have full body motion tracking, and it is currently an issue that developers are starting to tackle. The HoloSuit[10] is an example of this type of technology. It is a smart track suit with sensors embedded in it to track the user's movement, but it isn't yet available

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[10]http://kaayatech.com/ [accessed: 13/12/2017]

Figure 2.15: PrioVR on the left and VicoVR on the right

for sale. Another example is the Perception Neuron, which is a system based on individual tracking sensors called Neurons. These sensors are light-weight and small, adding no extra effort from the user to wear them, and they can be placed where they are needed to capture the level of detail and body movements that it is required for the project. PrioVR[11] is a also a motion capture suit under development, which consists on a series of sensors strapped to the body that enables the skeletal movement to be accurately digitized. One example that is a little different is the VicoVR[12], a Bluetooth accessory that delivers wireless full motion an positional tracking to smartphone-powered virtual reality headsets. It allows users to move feely within mobile gaming spaces.

There are some more type of systems, this are just a few examples. One problem with some of these hardware devices is that they can be bulky, heavy and not very comfortable to use. Even though they can have good results and provide a great full-body immersion experience, the fatigue and effort factors can contribute to a short-lasting exposure.

2.5.3.4 Leap Motion

The Leap Motion sensor[13] is a device that detects and tracks the user's hands as well as the fingers. It uses infrared LEDs and two cameras and it's detection area is a roughly hemispherical area that extends to a distance of about 1 meter. This device can be used on its own for different applications, but it can also be used in virtual reality, since it has a VR Developer Kit that can be attached to any Windows VR headset.

This hardware is light-weight, easy to use and touchless, meaning that the user doesn't need to touch the device to perform an action. Although it has these advantages and can also give accurate information about the hands and finger, it does have some issues in detecting both hands. The main problem is that if the hands get to close to each other or overlap, the sensor can't properly recognized them, and it gets weird and unreal results from the detection.

Some studies have been made to analyze the performance of the Leap Motion in comparison with a regular mouse [20] [21], which show that, overall the mouse has better results in pointing, clicking

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[11]https://www.kickstarter.com/projects/yeitechnology/priovr-suit-up-game-on [accessed: 14/12/2017]
[12]https://vicovr.com/ [accessed: 14/12/2017]
[13]https://www.leapmotion.com/ [accessed: 9/12/2017]

and positioning tasks. There are also some feedback issues that need to be taken into account, since unlike the gloves-type hardware which can give haptic feedback, this sensor doesn't have that capacity. This problem was seen in a study comparing touch and mid-air gesture input [22]. However, most of the tests performed used a 3D environment, but not within virtual space, meaning that they didn't use virtual reality in these tests. There aren't many studies or tests made with the Leap Motion sensor in a virtual world, although it's characteristics makes it suitable to do so.

Figure 2.16: Headset Vive with mounted Leap Motion sensor on the left and Leap Motion Controller on the left

3

Concept

Contents

This chapter focus on the conceptual implementation of the game. Concepts that were presented in the Background chapter will be correlated with the game concepts and mechanics.

3.1 Idea

The first component to be set was the chemistry domain in which the game should focus. Initially, it seemed like it would be a fairly quick and easy decision because of the target audience of the game and the context in which the game is supposed to be used. The target audience are high school students and the game is supposed to be used within the class as a complement to the learning process. These aspects help to restrict the scope of the domain to the subjects that are taught to high school students on Organic Chemistry.

However as it was detailed in section 2.1.2, high school students learn a variety of subjects related to Organic Chemistry but this game will focus on the objectives that encapsulate the basic knowledge that a student should acquire. This corresponds to the subjects that are taught to freshman students. After researching and also talking to teacher Antónia Gomes, a high school Chemistry teacher from Escola Secundária Raúl Proença, the defined domain of the game includes the nomenclature, structural drawings and functional groups of organic molecules. With the help of the teacher, the different subjects were explained in detail, particularly what are the most relevant concepts that the students should learn from each one and what they should be able to do.

The several parts of the domain are integrated in the different game modes available on the game. Initially there were only two main game modes defined which were the Normal and the Speed Run modes. Both of them use the domain in it's full scope, meaning that they have different types of challenges related to each part of the domain. These game modes will be detailed in section 3.5

In the last revision of the general idea, there were four more game modes included. These are sub game modes that focus on the different types of challenges that the game has, which means that each mode only presents one type of challenge. Therefor these sub game modes are Build, Complete, Transform and Multiple Choice. These types of challenges will be described in section 3.4

The game mechanics used in all of the game modes are the same, making it easy for the player to switch between modes without having to adapt to different mechanics. The player can **create molecules by connecting the atoms** and he can **translate** and **rotate** the molecules. To connect two atoms, the player must keep in mind the rules that exist in Chemistry related to this component, which are: the valence electrons each atom has available (detailed in section 2.1.1.3) and the functional group the molecule belongs to (detailed in section 2.1.1.4).

3.2 Conceptual Map

The figure 3.1 presents the concepts of the domain within the game and the relationships between them.

All the elements represented on the figure are implemented in the game, some have a physical representation and other are represented in the challenges. The ones with a physical representation are the atoms, molecules, valence electrons and the atomic size. This implementation will be explained in the Implementation chapter.

The functional group to which each molecule belongs to is integrated in the challenges of the game, as well as the name, formula and structure of the molecule. These are concepts that are used as information for the players to solve the different challenges.
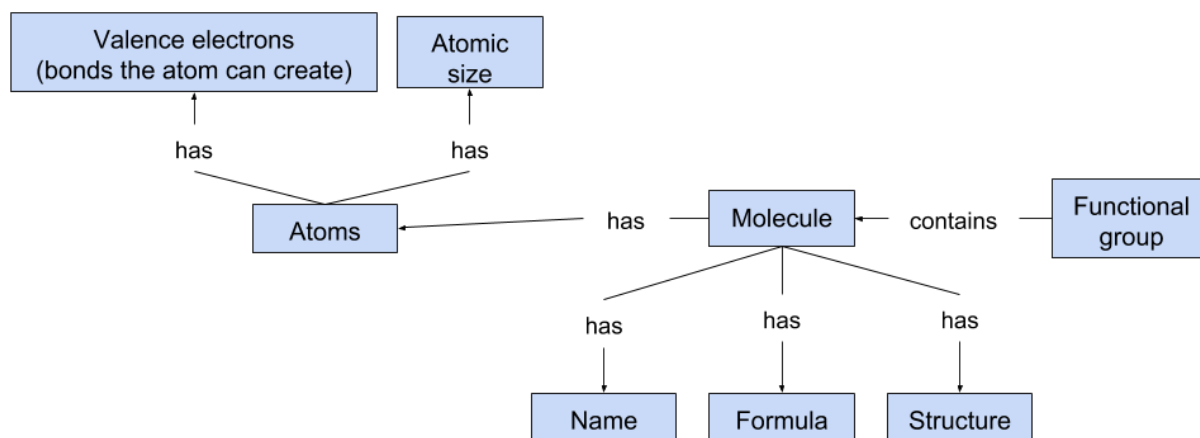
Figure 3.1: Conceptual Map of domain concepts

The figure 3.2 presents the concepts that exist within a single level and the relationship between them.

One level has one or multiple tasks or challenges, which can be of different types: Build, Complete, Transform or Multiple Choice (they are further detailed in the section 3.4). Depending on these challenges, there are two routes: one where he explicitly manipulates a molecule and the other where he answers a question. If he has to explicitly manipulate a molecule, when he finishes, he presses a button present in the scene to check if it is correct. If it is, the number of moves he made is checked and the points he deserves according to that number of moves is given. However if it isn't, he needs to go back and rebuild the molecule. On the other hand, if the player needs to answer a question, if he answers correctly, the number of attempts he made is checked in order to give him the appropriate number of points. If doesn't guess correctly, he needs to keep trying until he selects the correct answer.

The figure 3.3 represents the different manipulations that can be done with a molecule and with the atoms. From a box of atoms, the player can pick up as many as he wants, he can connect them together.
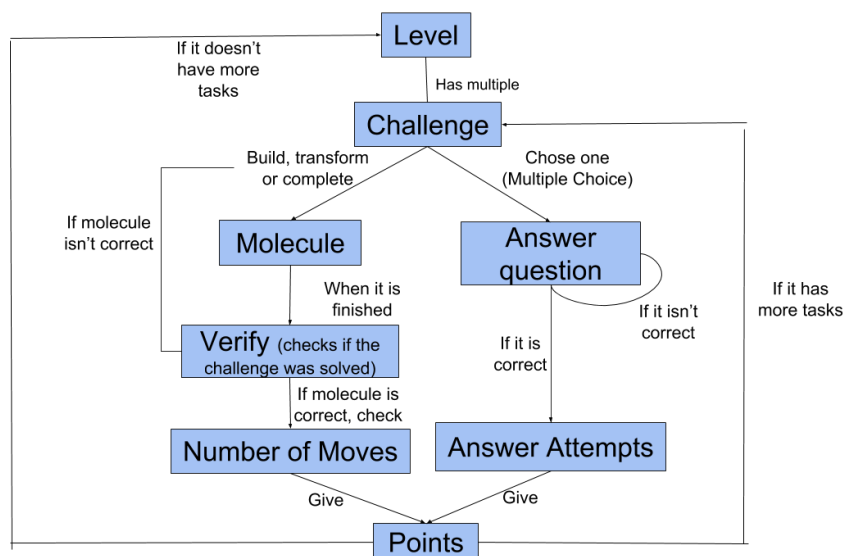
Figure 3.2: Conceptual Map of a level
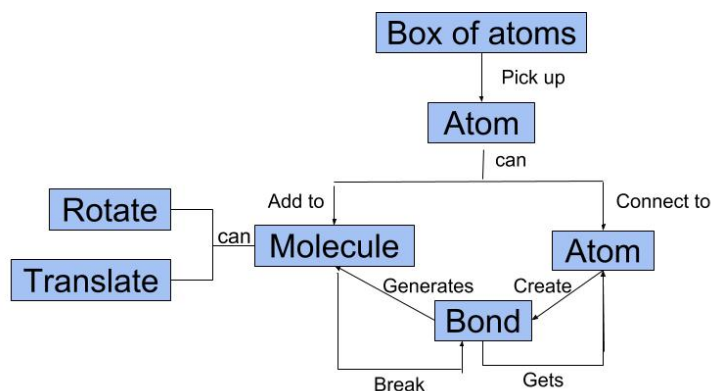
Figure 3.3: Conceptual Map of manipulating a molecule

When he connects them, a bond is formed and consequently a molecule is generated. However, he can also add atoms to an existing molecule. The molecule can be rotated and translated through methods that will be further explained in the Implementation chapter. He can also break a bond between two atoms.

3.3 Learning goals

Since the game has a strong educational aspect, one of the most relevant components to define are the learning goals. These must clearly define what the users should learn about the domain through the game. This means that the game must provide the means to reach the learning objectives.

After an initial research, these goals were based on what the students learn about the domain and

were some general goals. However, as it was mentioned previously I had the opportunity to talk with teacher Antónia Gomes, and after this talk the objectives were updated and became clearer because there were some of them that were a bit harder to fully understand for someone who isn't very knowledgeable in Organic Chemistry.

The final learning goals defined are:

- Recognize and name the major functional groups (hydrocarbons, carboxylic acids, haloalkanes, alcohols, aldehydes and amines)

- Recognize the functional group a molecule belongs to

- Know the nomenclature of the molecules (the nomenclature of a molecule is detailed in the section 2.1)

- Correlate molecular structure with the nomenclature

- Correlate conventional drawings of molecular structures with their 3D structure

The updates to the initial learning goals were to remove some of them that weren't taught in freshman year in high school, such as organic acids and bases, isomerism and reaction mechanisms. Also, some were split into several objectives, for example, learning the functional groups was slip into recognizing and naming them, and recognize the functional group a molecule belongs to.

3.4 Challenges

The game begins in the main menu, which will be detailed in the Implementation chapter, where the player can chose between two modes, Normal and Speed Run, which are explained in the section 3.5. Both of these modes have several levels which have different challenges that the player has to overcome in order to progress in the levels. The goal of the player is to reach the last level of each mode with the best score possible. The way the scores are implemented is explained in the section 3.5 as well.

There are four different types of challenges that the player is faced with, which are:

- **Build molecule from scratch knowing some information about it** (Build) - the player has to connect the atoms to build the molecule with only a piece of information about. This information can be anything about the molecule, it can be the structure, the name, the functional group it belongs to or the formula;

- **Complete a given molecule knowing some information about it** (Complete) - this challenge is very similar to the Build challenge, the difference is that instead of building the molecule from scratch, the player has a partially built molecule that he must complete, considering the information

that is given. The partially built molecule doesn't need to be altered, apart from adding more atoms to it, since it will not be shown a molecule that isn't correct according to the question;

- **Multiple choice question** (Multiple choice) - in this challenge the player has to answer a question about the molecule that is placed in front of him. The question has 3 possible answers and the player has to look at the molecule and figure out what the correct answer is.

- **Transform a molecule into another** (Transform) - for this challenge, the player is faced with a complete molecule and information about the molecule that he must achieve. The objective is to transform the given molecule into a molecule that corresponds to the information that is given. This information can be the name, the functional group, the formula or the structure of the intended molecule.

The four types of challenges were initially defined to directly correlate the initial learning goals. However, after the final learning objectives were settled and also after talking with teacher Antónia Gomes, the way the challenges were to be used was modified. One of the things that was discussed were the exercises that were applied to this subject and how they are used to solidify the concepts that the students learn. It was clear that the same type of exercise can be used for different concepts, for example, a multiple choice question can be made to determine which functional group a molecule belongs to, or what is its name, or their structure. With this in mind, the challenges no longer directly correlate with the learning goals, each challenge can be adapted to each learning goal. This means that the same challenge can be used for different learning objectives, making them versatile. This way, these challenges can be used in any subject of the domain, and are not restricted to one single learning objective. The figure 3.4 reflects this aspect, where one learning goal can be used with the different challenges.

Learning goal - Know the nomenclature
The nomenclature is methane.
Challenge Build - Build a methane molecule
Challenge Complete - Complete the molecule knowing it is methane
Challenge Transform - Transform the molecule into methane
Challenge Multiple Choice - What is the name of the molecule?
a. Methane
b. Ethane
c. Propane

Figure 3.4: Example of the same learning goal with different challenges

3.5 Gameplay

As it was previously said, there are two main game modes, Normal and Speed Run, that use the domain in it's full capacity.

3.5.1 Normal Mode

The Normal mode is a slow paced game mode and focus on the player having time to learn and absorb the knowledge. In this mode, there are 50 levels and each level has challenges. One level can have multiple challenges of the same type, or it can have challenges of different types.

The difficulty in this mode can vary in two distinct ways. On one side, the levels can be more difficult according to how many learning goals they tackle. A level that focuses on only one learning goal will be easier to surpass than a level that mixes two or three learning goals. On another hand, the challenge types don't have the same difficulty range amongst themselves, and also a single challenge type can be more or less difficult according to what it asks to do.

With this in mind, the difficulty for this mode will get increasingly harder in both the levels and the challenges. The first 20 levels tackle a distinct learning objective at a time, meaning that there are 4 levels per learning goal, as it showed in the figure 3.5.

Levels 1 to 4 - Know nomenclature of molecules
Levels 5 to 8 - Correlate molecular structure with nomenclature
Levels 9 to 12 - Correlate conventional drawings of molecular structure with their 3D structure
Levels 13 to 16 - Recognize the major functional groups
Levels 17 to 20 - Know the major functional group a molecule belongs

Figure 3.5: The first 20 levels of the Normal game mode with their correspondent learning goal

The order of the learning objectives is correlated to the order in which the students learn the different concepts in class. This way, the progression of difficulty of the subject tackled will be the same as it is presented in class by the teacher.

As it was said previously in section 3.4, each challenge can be used for all learning goals, and because there are 4 different types of challenges (Build, Complete, Transform and Multiple Choice), the first 20 levels apply each challenge to each learning challenge. The figure 3.6 represents the structure of the levels divided by the challenges they have (for these 20 levels, each one has only one challenge).

With this structure, the player is introduced to the different types of challenges within each learning objective, so that he doesn't associate a specific type of challenge to one learning goal. This is important to mitigate a learning effect on how to solve the challenges, because if the same type of challenge is always presented within the same context, the player won't need to think too much on how to solve it. The primary goal is to get the player to think about what it is asked and how he can solve the challenge

Level 1 - Build	**Level 5** - Build	**Level 9** - Build
Level 2 - Complete	**Level 6** - Complete	**Level 10** - Complete
Level 3 - Multiple Choice	**Level 7** - Multiple Choice	**Level 11** - Multiple Choice
Level 4 - Transform	**Level 8** - Transform	**Level 12** - Transform
Level 13 - Build	**Level 17** - Build	
Level 14 - Complete	**Level 18** - Complete	
Level 15 - Multiple Choice	**Level 19** - Multiple Choice	
Level 16 - Transform	**Level 20** - Transform	

Figure 3.6: The first 20 levels of the Normal game mode with their correspondent learning goal

with the knowledge that he has, and a way to achieve this objective is by giving the player the different challenges in different contexts. This will push the player to be constantly thinking and actively process his knowledge to figure out the best way to solve the challenge.

The next 15 levels mix two learning objectives and the last 15 levels mix three learning objectives. Besides this evolution, the challenges within each level also get increasingly difficult with what they ask the player to do.

1. Recognize and name the major functional groups
2. Recognize the functional group a molecule belongs to
3. Know the nomenclature of the molecules
4. Correlate molecular structure with the nomenclature
5. Correlate conventional drawings of molecular structures with their 3D structure

Level 21 to Level 23 - 3 and 4	**Level 33 to Level 35** - 2 and 5
Level 24 to Level 26 - 1 and 2	**Level 36 to Level 40** - 1, 2 and 3
Level 27 to Level 29 - 1 and 3	**Level 41 to Level 45** - 3, 4 and 5
Level 30 to Level 32 - 4 and 5	**Level 46 to Level 50** - 2, 3 and 4

Figure 3.7: The remaining 30 levels and the learning goals each tackles

For these last levels, the challenges are not specified because they would require more discussion with professor Antónia Gomes in order to understand how the challenges should be to achieve the intended learning goals. It wasn't possible to have this discussion due to conflicting schedules from both parties.

3.5.2 Speed Run Mode

The Speed Run mode is a fast paced game mode and it emulates a quiz, where the player has a time limit to complete all the challenges he is faced with. In this mode, there are 10 levels, each level with 5 challenges that the player must solve as fast as they can.

The difficulty in this mode progresses differently from the Normal mode. All the levels tackle a distinct learning objective at a time, meaning that there are two levels per learning goal. The first level of each learning goal has easier challenges and the second level has harder challenges. This means that the difficulty for this mode isn't has high has the Normal mode, particularly for the levels.

The order in which the learning goals are faced by the players is the same as in the first 20 levels of the Normal mode.

3.5.3 Scoring System

The scoring system of the game is based on two measures: number of attempts and number of moves. They are not used at the same time, it is only used one or the other, and the decision on which one should be used is based on the game mode and on the challenge type. The initial idea was to use time instead of the number of attempts, but this method wouldn't be fair to the players. If one took more time to answer and selected the correct answer on the first try, he would be penalized, while a player that would guess at random without thinking could select the correct answer faster. For this reason, this scoring method was removed and replaced.

In the Normal mode, the skill of the player is measured in number of moves for the challenges Build, Complete and Transform because these challenges force the player to manipulate the atoms and interact with the molecule to solve them. For this reason, it makes more sense to count the number of moves that the player performs until he reaches the desired molecule, instead of time (as it seemed like a viable scoring method at first). In these challenges, if the molecule is more complex, it is normal to take more time to built it and if the player is scored by the time, he might try and rush through the interactions and fail mores times, causing frustration. To avoid this, it was decided that the number of moves would be a more suitable choice. For a Multiple Choice challenge it doesn't make sense to rate the skill of the player by the number of moves that he makes to complete the challenge, because it isn't necessary for him to interact with the molecules as much as in the other challenges. Instead the player is rated by the number of attempts he makes until he selects the correct answer.

In the Speed Run mode the skill of the player is measured only in time, since the only thing that matters is how fast the player can finish all the levels. In this case, to mitigate the possibility of frustration happening when solving the challenges Build, Complete and Transform, these challenges will be as simple as possible. The challenges Build will only have simple molecules to build with one or two carbon atoms in the main chain. The challenges Complete will present molecules 75% built, so that the player has few atoms that he needs to add to it to complete it. And finally, the challenges Transform will also be simple molecules, with few atoms to take out and add, making this challenge quicker to solve.

3.6 Environment

The environment is very simplistic but appealing to the user. It is inspired in class rooms and labs, in order to promote the feeling of being in a suitable environment to manipulate atoms and molecules. Most objects in the scene have a purpose to them, besides adding to the intended environment it also has an usefulness for the challenges. An important aspect that was defined from the beginning is that the player has to be able to interact with the setting in fun and entertaining ways, even with some objects that don't have a major importance in the gameplay.

4

Implementation

Contents

This chapter corresponds to the technical implementation of the game with the respective development iterations and its progress, testing, critics, decisions and justifications.

The game was developed with HTC Vive and Leap Motion sensor. It was used the Leap Motion Orion SDK[1] which was built specifically to be used with virtual reality. It was also used Steam VR with the HTC Vive, which was launched with native support for Unity on its platform.

The development of the game was initially divided into two different stages, the first one would focus on the implementation of the core mechanics and the second on the gameplay and overall look of the game. Each phase would have a testing session to evaluate the progress made and from the results of the test the game would be improved. This way there would be feedback throughout the development process, instead of only at the end, and it enables immediate improvement on each implementation phase. With this method, it mitigates the need to modify a component on a later stage that could drastically change everything else that was implemented on top of it, and potentially causing more problems.

This initial plan was slightly changed with the addition of an extra phase between the first two stages. This intermediate stage was added because the results from the first phase weren't conclusive enough to be able to progress to the gameplay implementation stage. In this intermediate phase the focus was still on the core mechanics, improving them according to the results from the first iteration, and then testing them again.

The figure 4.1 represents a timeline of the development iterations with the different stages.

	February		March				April					May			
Iterations / Week start day	19	26	4	11	18	25	1	8	15	22	29	6	13	20	27
1st Iteration															
Implementation															
Tests															
Analyse results															

	June				July		
Iterations / Week start day	3	10	17	24	1	8	15
2nd Iteration							
Implementation							
Tests							
Analyze Results							

	July		August				September					October		
Iterations / Week start day														
3nd Iteration	22	29	5		12	19	26	2	9	16	23	30	7	14
Implementation														
Organizing tests on school														
Tests														
Analyze Results														

Figure 4.1: Development iterations timeline.

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[1] https://developer.leapmotion.com/orion/#105

During the month of August the focus was only on writing the report.

In this first stage, the goal was to create the core mechanics that involved the manipulation of objects in Virtual Reality. These core mechanics were connecting atoms, rotating molecules and translating molecules. The first mechanic to be implemented was connecting atoms together since this is the way to create molecules and therefor the most important mechanic to implement. The translation of molecules was the second mechanic to be developed because out of the remaining mechanics, this one posed the smallest challenge to implement. And finally, the rotation of molecules was implemented and, as expected, it was the most difficult mechanic to implement.

4.1 First development iteration

This iteration corresponds to the initial development of the game. In this iteration, the atoms could be connected and the bonds between them could be broken. The molecules created could be rotated and moved as a whole.

The overall environment was simple and had basic objects, since the focus was on the interaction with the molecules instead of the general look of the game.

Relationship between an atom and a molecule

There were a lot of aspects that were defined in this stage that impacted the later development of other components. One of the most relevant was the relationship between an atom and a molecule as objects in the game.

When two atoms are connected, a bond is created between them and a molecule is formed. The molecule is the parent object of both atoms and the bond. Every molecule has a pivot, which is a small sphere that represents the center of the molecule. The position of the pivot is the mean of all the atoms position with an offset on the y axis, which means the pivot appears always slightly below the molecule. Because the position of the pivot depends on the position of the different atoms, it is constantly updated according with the positions of each one.
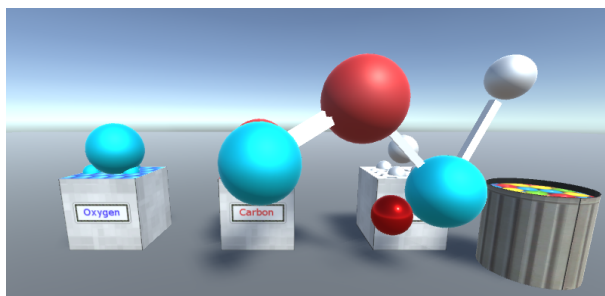
Figure 4.2: Example of a molecule (the pivot is represented by the smallest red sphere).

4.1.1 Interactions

The other important aspect that was defined were the methods of manipulation of the molecules. One of the main objectives for all the types of manipulation of the molecules was to have a natural, intuitive and easy to use interaction. With this in mind, in this first iteration, multiple ways of performing the same type of interaction were implemented and later tested.

Connecting atoms

This mechanic is strongly connected to the domain of the game, because the way the atoms should be connected is directly related to the valence electrons each atom has and consequently the bonds they can form with each other. Each atom type has a different number of valence electrons which are connected the number of bonds it can have (see section 2.1.1.3). For example, an Oxygen atom has 2 valence electrons which means that it can two simple bonds with other atoms, or a double bond with another atom. For a molecule to be correctly built, all atoms mustn't have any free valence electrons, meaning that it shouldn't be possible to add any more bonds to the molecule.

Initially there was only one method that was implemented which was through tapping two atoms to each other. Each time the atoms are tapped to each other, the type of bond increases, beginning at a single bond all the way to quadruple bond. When it reaches to the triple bond, and the atoms are tapped again, it circles and goes back to a single bond. The figure 4.3 represents the tapping method as it was explained. The small dots next to each atom represent its valence electrons, and when the player let goes the atoms, they disappear according to the bond he made. In this figure, he made a double bond, meaning both valence electrons from the atoms were shared and so, the small dots that represented those valence electrons are removed.

After some discussion about how the atoms should be connected, it was decided to implemented a different technique which was through distance. In a similar way as the tapping method, the atoms are tapped into each other but only once. After they are tapped, the player defines the bond he wants to create by moving the atoms away or closer to each other. The closest the atoms are, the stronger is the bond type and the farthest the weaker is the bond. This method was created to simulate in some way the forces of repulsion and attraction between the different atoms.

Translation

To move the molecule into a different position, the player could use two different ways. One method was to grab one of the atoms of the molecule and move it to the desired location and the rest of the atoms would be dragged along. The other method was to grab the pivot with his left hand, and move it, which would make the whole molecule move without losing its shape.
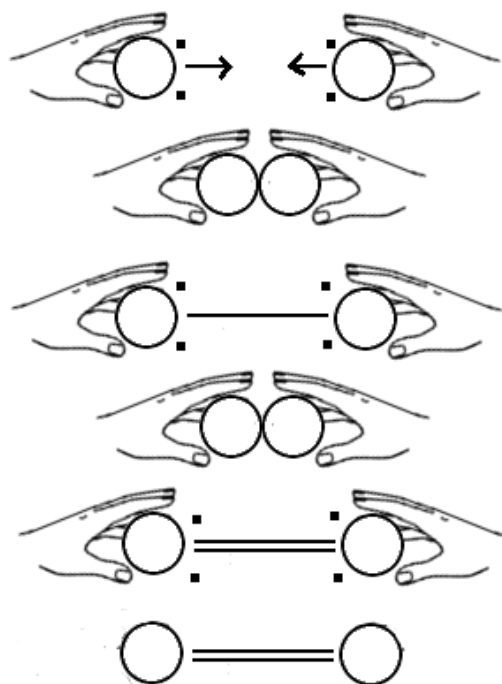
Figure 4.3: Example of connecting two atoms through the tapping method.

Rotation

For the rotation, there is one aspect that is present in all methods, which is that the user must grab the pivot of the molecule with his right hand. This activates the rotation mode.

There is another aspect that is only present in the methods where it is necessary to set the rotation axis, which is the way that this axis is defined. Since the right hand of the user already has a purpose, the left hand is responsible for this part. There are two different methods that allow the player to set the rotation axis. Both of them use two distinct hand gestures, which are showed in the figure 4.4.
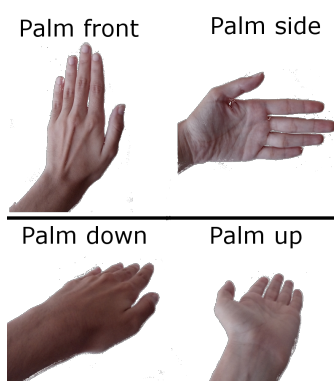
Figure 4.4: Hand gestures for setting the rotation axis (each method is represent in each row).

The hand gestures of Palm front and Palm Up set the Z axis while the Palm Side and Palm Down

gestures set the X axis.

These two techniques to define the rotation axis were tested along side the rotation methods. There were three different methods implemented:

- *Automatic rotation* - in this method the player only needs to grab the pivot of the molecule with his right hand and define the axis around which the molecule should rotate with his left hand. He can set one of two axis, the X-axis and Z-axis, through two distinct hand gestures which vary according to the method being used (showed in figure 4.4). After the pivot is grabbed and the axis set, the molecule rotates on its own.

- *Rotation with wrist control* - for this method, it is also necessary to define the axis around which the molecule should rotate through the same gestures explained in the Automatic rotation.

  However, in this technique the molecule doesn't rotate on its own. The rotation of the molecule is controlled by the rotation of the right wrist, this means that the player has to grab the pivot of the molecule and while grabbing it, he must rotate his wrist to rotate the molecule. The movement that the wrist must do is very similar to the movement a person has make when unlocking a door with a key.

  While the user rotates the wrist, the value of the current rotation is stored as well as the value of the last rotation, both of these values are in angles, and the difference between these values is sent to the molecule, where an offset is also applied. The current and last rotation are updated on each frame, causing the difference between them to be very small. For this reason, when the difference is added to the molecule to make it rotate it translates into a small rotation on the molecule. This issue made the method challenging to implement because it is necessary to correlate the rotation of the wrist with the rotation of the molecule. Both should be synchronized to make the interaction as natural and smooth as possible. An offset was added to the difference in the rotations as a way to solve this issue. The value used for this offset was 3.5 which was found after some trial and error.

- *Rotation with atom* - in this technique it isn't necessary to define any axis. The player has to grab the pivot with his right hand and grab one atom of the molecule with his left hand, and then he has to move the atom around what would be the center of the molecule. When he begins to move the atom, the pivot no longer has the offset on the y axis and it appears in the center of the molecule. This way the player has a visual reference of where it is, making it easier to understand how he must move the atom to rotate the molecule around the central point. As the atom is moved around the pivot, the whole molecule follows its movement, making it rotate around the pivot.

Other components

Besides these components, this iteration also had a shelf that was used to save molecules and the player could also load them whenever he wanted. This was created with the later intentions to use it to store molecules in each shelf by their class or number of carbon atoms, for example.

4.1.2 Test

In this stage of development, it was decided that the different types of interactions should be tested because there were multiple methods that could be used in each interaction, and it was necessary to understand which one should be used. The choice of the best one to use was made based on their ease of use, their efficiency and is less prone to make the player cause mistakes.

The test had three parts, one regarding the rotation, another for moving the molecules and another one for connecting the atoms.

The rotation part had only one task that the users should perform, which consisted on rotating a given molecule to reach a final rotation which was shown to the user as see-through molecule. However they were asked to perform it with all three rotation methods and also the two methods to define the axis. This means that the user had to perform this task 5 times, always with the same final position and the same molecule.

In similarity with the rotation part, for moving the molecules, the user was also faced with one task, which was to move a given molecule to a final position that was shown to the user as a see through molecule. They had to perform this task with the two different methods implemented to move a molecule.

In the part related to connect atoms to create molecules, the user had 3 tasks to perform, which were performed with the two methods created to connecting atoms.

- Create a single bond between two atoms of Carbon

- Create a triple bond between two atoms of Carbon

- Create a double bond between a Carbon atom and a Oxygen atom, and a single bond between the same Carbon atom and a Hydrogen atom.

4.1.3 Experimental method

During the test, there were some logs recorded to be able to measure efficiency and effectiveness in each task. These logs saved the time that each user took to complete each task with each technique implemented and also the number of times the users needed to reset the task. The recorded value of time would be used to analyze the efficiency in each task and the number of resets would be used to evaluate the effectiveness.

At the end of the test the users were asked to fill a questionnaire about the tasks they performed and it also had a few questions based on the VR Sickness questionnaire, in order to figure out if they

felt uncomfortable during the session. The questionnaire was divided in 5 parts, as it can be seen in appendix A.1, the first one is general information about the individual and his experience with Virtual Reality technology, the next three parts are about each of the three types of interaction with the molecules, and the last part is about VR Sickness.

Rotation section

For the questions related to the rotation techniques, the users were asked to put in order of least to most each of the techniques according to their complexity, intuitiveness and ease of use. For this reason, the method used to analyze the results was Weighted Sum, where there was a weight associated to each position in the order. These weights were attributed accordingly to what was the best position and the worst, the best has the biggest weight and the worst has the lest weight.

In the first question, the users were asked to order the techniques from least to most complex, meaning that the technique placed in first place was considered the least complex, and the technique placed in third was considered the most complex. This way the first position had a weight of 3, the second of 2 and third of 1.

For the other two questions, the weight distribution the reverse of the first question. The first position had a weight of 1, the second of 2 and the third of 3, because a technique that was placed in first was considered the least intuitive and least easy to use, and the technique that was placed in third was considered the most intuitive and the most easy to use.

There were also questions regarding the method to define the rotation axis. These questions were more direct, they were all to chose between the two, which one was the one they preferred. One question was about which method was the easiest to define the axis and the other question was about which one was the most intuitive. These two questions were made regarding each rotation technique that needs the rotation axis to be defined, which are the method Automatic and the method Rotation with Wrist Control. This helps to see if there are differences in using the two methods for different rotation techniques or if it is independent to the way that the molecules are rotated.

Translation and connecting atoms section

These two sections had similar questions and the same method of analyzes applied to them. The questions asked to the users were about complexity, intuitiveness, ease of use and preferred method. For each question, the users had to chose, from the existing techniques, which one they thought was the better than the other. Each type of manipulation had two techniques implemented and tested. This means that the users had to chose which of the two techniques implemented for translation was the most complex, the most intuitive, the easiest to use and the one they preferred, and the same for the two techniques implemented for connecting atoms. The analyses of the results was made through

percentages of each answer.

4.1.4 Results

There were 18 users for this test, 15 male and 3 female, where 12 of the subjects had already had contact with some type of Virtual Reality technology and 6 of them had not. All of the experiences they had with Virtual Reality were through games and simulations. In the Rotation section there are only 17 responses because one of the users couldn't perform any of rotation tasks due to some problems in the code that were quickly resolved.

1. Rotation section

In the figure 4.5 we can see the results and the analyses done.

Question complexity								
	First	First*3	Second	Second*2	Third	Third*1	Sum	Average
Automatic	9	27	6	12	2	2	41	2.411764706
Wrist	2	6	5	10	10	10	26	1.529411765
Atom	6	18	6	12	5	5	35	2.058823529
Question Intuitiveness								
	First	First*1	Second	Second*2	Third	Third*3		
Automatic	4	4	8	16	6	18	38	2.235294118
Wrist	5	5	7	14	5	15	34	2
Atom	8	8	6	12	3	9	29	1.705882353
Question Ease of use								
	First	First*1	Second	Second*2	Third	Third*3		
Automatic	7	7	4	8	6	18	33	1.941176471
Wrist	4	4	8	16	5	15	35	2.058823529
Atom	6	6	5	10	6	18	34	2

Figure 4.5: Analysis of the answers of the questions related to the rotation techniques.

For the question of complexity, the method Automatic had the highest average ranking out of the three methods. Also the sum of the weighted ranks indicate that the method Automatic was voted the least complex from all three. From this, the conclusion is that the method Automatic is the least complex method of the three.

Regarding the question about which one is the least intuitive and which one is the most intuitive, the method Automatic had the highest average ranking. Contrary to the complexity question, the weighted sums were not so disparate, they had values very close to each other, with method Automatic having a weighted sum of 38 - which was the highest - and method Atom having a weighted sum of 29 - which was the least. After performing a ANOVA comparison with the weighted values, the result p value is 0.0261, which indicates that, even though the values are similar and close to each other, there is still a significant difference between them to assume that the method Automatic is the most intuitive.

The last question which was about easy of use had very similar results as the question about intuitiveness. The highest average rank belongs to the method Wrist Control, but the difference between the three methods isn't very large. The weighted sums were also very close to each other. The highest weighted sum was 35 for method Wrist Control, and the lowest weighted sum was 33 for method Automatic. After performing a ANOVA comparison with the weighted values, the result p value is 0.0069, which indicates that, even though the values are similar and close to each other, there is still a significant difference between them to assume that the method Wrist Control method is the easiest to use.

In the figure 4.6, it is possible to see the results from the questions regarding the techniques to set the rotation axis.

Easy to use	Automatic	Wrist		Intuitive	Automatic	Wrist
Up / Down	58.80%	58.80%		Up / Down	58.80%	47.10%
Front / Side	41.20%	41.20%		Front / Side	41.20%	52.90%

Figure 4.6: Percentage of users that chose each method for the two questions.

For both rotation techniques, the method of Palm Up Palm Down had 58.8% of votes as the easiest to define the rotation axis. For intuitiveness, this method had also 58.8% of votes for the method Automatic, but for the method Wrist Control, it dropped to 47.1%. This means that 8 people chose the Palm Up Palm Down method, and 9 people chose the Palm Front Palm Side method, making it indifferent the most intuitive method for this rotation technique. Overall, the conclusion is that the best method chosen was Palm Up Palm Down.

The last question regarding the rotation interaction was asking what method the users liked to use the most, and the two most answered methods were Automatic and Atom. The reasons given for the method Automatic being the most liked were that the technique was working the best, having immediate feedback and being intuitive. For the method Atom, the reasons given were that it provided the best control, worked better and it was interesting and intuitive.

2. Translation section

In the figure 4.7 it is possible to see the results of the questions asked about the translation techniques.

The technique of moving the molecule by grabbing the atoms was indicated as the most intuitive by 14 users (77.8%) easiest to use by 13 users (72.2%) while the method of moving the molecule by grabbing the pivot was the most complex by 15 users (83.3%) as it can be seen in the figure 4.7. Overall, the method of moving the molecule by grabbing the atoms was preferred, with 77.8% of users indicating that they would like to use it.

3. Connecting atoms section
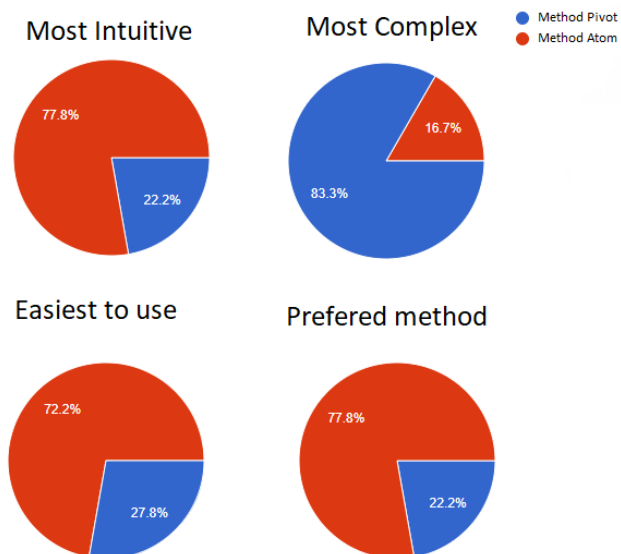
Figure 4.7: Pie charts with the answers to the questions about the movement techniques.

From the figure 4.8, we can see that, out of 18 users, 66.7% claim that the tapping method is easier to use, 66.7% say that it also is the most intuitive and 38.9% indicate this technique as the most complex. Overall, 77.8% of the users prefer to use the tapping method over the distance method to connect atoms and form molecules.
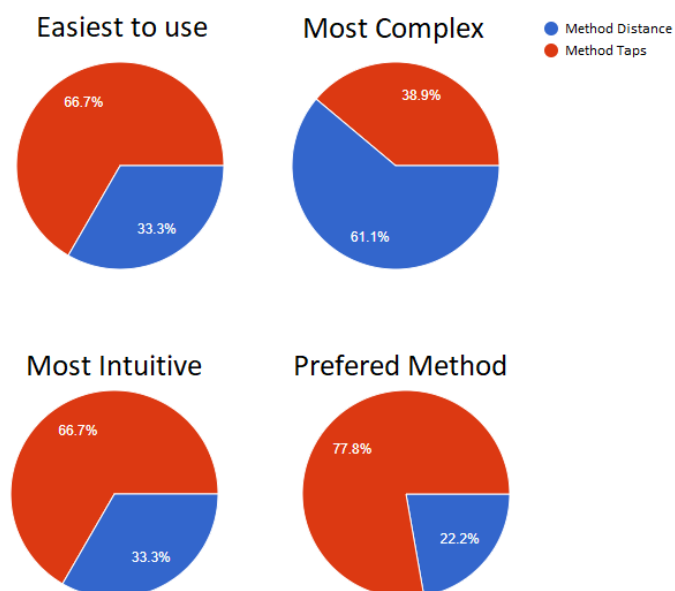
Figure 4.8: Pie charts with the answers to the questions about the connecting atoms techniques.

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4.1.5 Problems

With this test, it was possible to discover some problems that some methods had that were not visible during their initial implementation. Some problems were big enough to make the technique not work properly, and thus having a significant influence on the answers the users could give. For this reason, as soon as the problems were seen, they were resolved.

Despite the major issues being solved, some techniques, particularly the Rotation with Atoms and the Wrist Control which are methods of rotation, had flaws that could be improved. This caused the majority of users (5 out of 7 that chose it) to say that although they picked the Automatic Rotation method as their preferred technique, they said the they liked the others better. They chose the Automatic Rotation as the preferred one simply because it was the technique that was functioning better.

The biggest issue with the test itself was that the logs didn't save the times of each task properly. Most of the tasks appeared without any value for the time, and others showed an absurd value of almost 20 minutes to complete a task, which didn't happen. This made it impossible to analyze the techniques from the efficiency point of view. Also, the same issue occurred with the logs of the number of resets on each task, so the effectiveness of each task was also unevaluated.

The test didn't have any logs regarding the positions of the molecules, making it very difficult to know whether the users were able to complete the tasks successfully. For this reason, the results were only based on the answers given in the questionnaire and observation of the tests.

4.2 Second development iteration

In this stage of development, some changes were made according to the results from the test done in the first iteration. As it was mentioned in 4.1.5, two of the rotation techniques implemented, Rotation with Wrist Control and Rotation with Atoms, needed to be improved but they were the most preferred methods. Although the users chose the Automatic Rotation has their preferred technique, the majority of them mentioned that they only picked it because it was the one that was working with less problems, not because they liked it better. For this reason, the Automatic Rotation method was discard, and the focus on this second iteration was to improve the other two techniques and test them with proper logging.

Rotation methods

One of biggest problems in both techniques was the place that the pivot of the molecule appeared. For most molecules, the pivot was in a position that made it difficult to interact with them and perform a rotation or even a simple translation. Most of the times, the pivot was hidden by the atoms in the middle of a rotation or the user would have to place the hands in awkward positions to be able to perform the

tasks. Because of this, the position of the pivot was changed from being below the molecule, to appear to the right of the molecule.

Along side this problem of the pivot, another issue that was contributing to this predicament was the fact that the translation interaction and the rotation interaction were assigned to distinct hands - left hand to move, right hand to rotate. This made it hard to perform some tasks and even when it wasn't necessarily hard, it was observed that the users would try and use either hand to perform the tasks and they had a difficult time associating each hand to a separate type of manipulation. To mitigate this issue, the movement of the molecule was changed to be performed by either hand.

Another aspect that needed to be improved was the offset applied in the rotation of the molecule when the Rotation with Wrist Control technique was used. The users were having difficulty in rotating the molecule because the offset was too low, making the molecule rotate less than what their wrist was rotating. To eliminate this issue, the offset was changed to a higher value.

Connecting atoms and translating molecules

For connecting the atoms, the technique that uses distance was discarded, since the tapping method had the best results, and for the movement techniques, they were both kept. Regarding the techniques to move the molecules, although the method that uses the atoms to move the molecule was the one the users liked the most, it was observed that this might have been due to the tasks that were given. The users didn't have any task to move the molecule to a far away position, or move a big complex molecule, which makes it unnecessary to use the pivot technique. Since they would have to manipulate both complex and simple molecules in the final version of the game, none of the techniques were disposed.

Montra de Jogos

In this phase of development, there was an event at Taguspark in which students in the Game courses would showcase the projects that they had been working on through out the semester. This was Montra de Jogos (MOJO) and this project was also showcased there. With this in mind, some elements of design were added since up until this point, the background was empty and wasn't aesthetically appealing. The most relevant components added where two black boards that had a functional purpose along side the aesthetic one. They were created with the thought in mind of displaying useful information to the user.

Besides having an improvement in the scenery, there was also a need to create a tutorial to present at the MOJO because only the core mechanics were implemented and the game wasn't organized with levels and with different challenges. The tutorial created had 5 levels, but due to some problems with the transition from level 4 to level 5, the users could only reach up to level 4. Since this was a showcase with a lot of games being displayed and many people trying them, the tutorial shouldn't be too long as to not take too much time of each person. For this reason, the levels had simple challenges and most of them had only one challenge, as it can be seen in figure 4.10. The molecules used for in these challenges

47
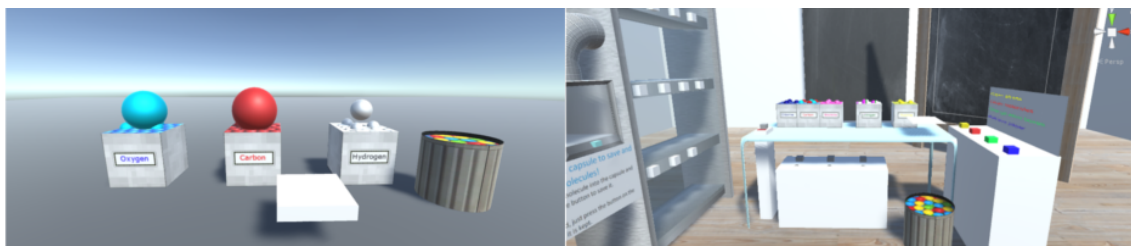
Figure 4.9: Game environment pre (left image) and post (right image) MOJO changes.

were not organic molecules because the audience that attended MOJO didn't have sufficient knowledge to be able to solve more specific tasks.

```
1: Build a H2O molecule;
2: Build a CO2 molecule;
3: Place the CO2 molecule in the position showed by the transluced molecule;
4: Save the CO2 molecule;
    Load the CO2 molecule;
```

Figure 4.10: Levels of the MOJO tutorial and their respective tasks

One of the boards that was added as part of the design, was used to display information about the current level and task at hand, and how far along the level the user is.

4.2.1 Test

In this iteration of development a test was made on the rotation methods, in order to define which one is the best and discard the other.

The test had 3 different task that should be performed with both rotation methods. The tasks all have the same objective, the user should rotate the given molecule in the final position displayed by a see through molecule. Each task has a different molecule, two of them are simple molecules and the remaining one has a more complex molecule. The tasks were presented in random order to the users to mitigate the probability of a learning effect occur.

4.2.2 Experimental method

On this test there were also logs that recorded information about each task to be able to analyze the methods according to their efficiency and effectiveness. In the logs is included the time the user took to perform each task and also the final rotation of the manipulated molecule on each task. These values of time on all tasks were compared according to the technique used, in order to check if there is a significant difference between them. There were also some other comparisons made to check if there is a significant difference in using one method before the other.

In similarity to the first test, there was a questionnaire at the end of it with questions about the tasks the users performed and it also had questions based on the VR Sickness questionnaire. The questionnaire was divided in 3 parts, as it can be seen in appendix A.2, the first one is general information about the individual and his experience with Virtual Reality technology, the next part is about the rotation methods and the last part is about VR Sickness.

In the questionnaires there were 3 different questions about the rotation methods, each of the questions is asked about both techniques. They were linear type scale where the users had to rank the techniques regarding their ease of use, precision and understanding how to use it on the first try.

4.2.3 Results

There were 10 users for this test, all male, where 8 of them had already been in contact with some type of Virtual Reality technology and 2 of them did not. All of the experiences they had with Virtual Reality were through games and simulations. From the 10 users, 7 had participated in the previous test.

In order to eliminate a possible learning effect between the techniques used, the first method used was changed for each user. The goal was to have half of the users using one method first, and the other half use the other method first. However, due to a mistake in checking the order with the last user, it ended up not being slip in half, having 6 users using the Rotation with Atom technique first and 4 users using using the Rotation with Wrist Control technique first.

The time the users took to perform each task with each method was recorded and analyzed from a statistic point of view.

Comparing the methods to each other without order of use

As it was mentioned in the section 4.2.3, some users used the method Rotation with Atom first and other used the method Rotation with Wrist Control first. In this section of the results, this order will not be taking into account in the comparison of the times recorded with each technique.

To compare the values record, the ANOVA with single factor test was used to check if there is a significant difference between the times recorded for the Rotation with Atom versus the times for the Rotation with Wrist Control (figure 4.11). The results indicate that the F value is greater than the F critical value and the p value is less than 0.05, which means that there is a significant difference between the groups. From the averages, it is possible to see that the users spent less time when using the Rotation with Atoms method in general.

Comparing the methods to each other with order of use

In this section of the results, it is checked if the order in which the methods were used has a significant different in the values of time recorded. For this reason, the order of use will be taking into account in the comparison of the times recorded with each technique.

Tester/Task	Pivot 1	Pivot 2	Pivot 3	Wrist 1	Wrist 2	Wrist 3
1	1.156651667	0.2885133333	1.233668333	3.327028333	2.94522	1.518923333
3	0.95057	1.065555	0.9504766667	1.579743333	1.081593333	2.373998333
6	0.652335	1.307751667	1.585926667	1.677283833	0.7600883333	1.859395
8	1.230716667	0.5836083333	1.524991667	3.370443167	1.01698	3.03056
2	1.219688667	2.617286667	1.609947833	8.18846	0.36336	5.778615
4	0.9774861667	0.8807131667	1.701466167	1.010263333	0.83285	1.478315
5	5.9445045	3.51113	1.37351	2.164833333	1.68749	5.06345
7	0.7478683333	0.2794433333	1.74911	1.081961667	0.9198233333	1.654975
9	2.492528333	1.933808333	3.677071667	1.16262	1.070406667	2.354083333
10	1.284305	0.9904283333	3.0458	2.533718333	1.880188333	5.299051667

Wrist - Pivot (rows 1, 3, 6, 8)
Pivot - Wrist (rows 2, 4, 5, 7, 9, 10)

Anova: Single Factor

SUMMARY

Groups	Count	Sum	Average	Variance
Pivot 1	10	16.65665433	1.665665433	2.515434976
Pivot 2	10	13.45823817	1.345823817	1.101063738
Pivot 3	10	18.451969	1.8451969	0.7165754183
Pulso 1	10	26.09635533	2.609635533	4.592885111
Pulso 2	10	12.558	1.2558	0.5428952066
Pulso 3	10	30.41136667	3.041136667	2.852938802

ANOVA

Source of Variation	SS	df	MS	F	P-value	F crit
Between Groups	25.63803	5	5.127607324	2.496847927	0.04175796938	2.386069853
Within Groups	110.8961	54	2.053632209			

Figure 4.11: Values recorded and statistic analyzes through ANOVA Single Factor test (Pivot - indicates the Rotation with Atom technique).

Also, a T-test was performed for the times of each method individually, comparing the values of when the technique was used first and when when it was used second. The method Rotation with Atoms had a value of 0.0054 and the method Rotation with Wrist Control had a value of 0.23091. These results show that the method Rotation with Atoms had a significant difference between being used first to solving the tasks or being used second. However, for the method Rotation with Wrist Control there isn't a significant difference between using it in first to solve the tasks or using it in second. This means that the method Rotation with Atoms sufers a learning effect.

Conclusions from the comparisons

From these results, it is possible to say that the method Rotation with Atoms has better results, even though there is a difference between using it first or second, while the technique Rotation with Wrist Control has worse results. Since the values of the Rotation with Atoms technique are always better than the Rotation with Wrist Control, the conclusion is that the Rotation with Atoms has better performance regarding the time spent to complete tasks.

Questionnaire analyses

From the analysis of the values through weighted ranks (figure 4.12), we can see that there aren't

big differences between the answers given to questions about the rotation methods. For ease of use, the Rotation with Atom technique had the highest value. By the sum we can confirm that there is a slight difference between both methods, with the Rotation with Atom technique having a bigger value.

In terms of understanding how to use the methods for the first time, the weighted ranks have the biggest difference. The Rotation with Atom technique has a bigger rank than the Rotation with Wrist Control technique.

For the question about precision, the Rotation with Atom method had the highest weighted average rank again, but similarly to the ease of use question, the difference between the two techniques isn't very big.

Easy

Value	#1	#1*5	#2	#2*4	#3	#3*3	#4	#4*2	#5	#5*1	Sum	Average
Method Wrist	1	5	2	8	2	6	4	8	1	1	28	2.8
Method Atom	2	10	3	12	1	3	3	6	1	1	32	3.2

Understand

Value	#1	#1*5	#2	#2*4	#3	#3*3	#4	#4*2	#5	#5*1	Sum	Average
Method Wrist	3	15	1	4	1	3	3	6	2	2	30	3
Method Atom	5	25	3	12	1	3	0	0	1	1	41	4.1

Precision

Value	#1	#1*1	#2	#2*2	#3	#3*3	#4	#4*4	#5	#5*5	Sum	Average
Method Wrist	3	3	2	4	2	6	0	0	3	15	28	2.8
Method Atom	1	1	3	6	1	3	4	16	1	5	31	3.1

Figure 4.12: Answers to the question about both methods

From these results, the conclusion is that the Rotation with Atom technique is considered better by the users, being the easiest to use, the most precise and the one that is easier to understand at first try.

4.2.4 Problems

Unfortunately, in these tests there were problems with the logs again. This time the issue was in saving the rotation where the users placed the molecule in each task, in most cases the rotation that was saved was not the rotation of the molecule that the users were manipulating. Instead the intended final rotation shown by the see through molecule was saved, which made the majority of the logs useless.

4.3 Third development iteration

In this stage of development the focus was on the gameplay, since up until this point the center of attention were the mechanics. Regarding the gameplay, in this phase the levels were implemented which includes all the different tasks, the ranking and evaluation systems of those tasks.

For the mechanics, based on the results of the test from the second iteration, it was decided to keep the Rotation with Atom technique and dismiss the Rotation with Wrist Control method.

Levels

One of the first components added was how to create the levels. In the previous state of development, detailed in section 4.2, was made a simple tutorial where there were simple levels hard coded into the game. In this phase, the levels were changed from hard coded to being flexible, allowing for easy changes in them without tempering with the code. The levels are now loaded from text files that must follow the structure indicated in the figure 4.13.

```
1: type of task..._ type of task...;
2: type of task...;
3: type of task..._ type of task..._ type of task...;
```

Figure 4.13: Template of the level's structure

Each level is differentiated by its number and each level can have multiple tasks. The different tasks within each level are separated by the character _ and the character ; is used to indicate the end of a level.

The tasks have their own specific name that must be used, or else the tasks won't be loaded correctly. Each task has its own structure because each has different components that have to be provided, as it is shown in the figures 4.14. These structures must be respected for the level to be loaded with no problems.

```
1 : multiple choice>question>molecule to display>correct answer
        >a.answer
        >b.answer
        >c.answer;
2 : build>molecule to build;
3 : complete>class & name or just class or just name>partial molecule to display;
4 : transform>molecule to transform;
```

Figure 4.14: Specific structure of each task

The figure 4.15 represents an example of 4 levels with different tasks, each with their respective structure.

```
1 : multiple choice >What is the name of the molecule?>CH4>a
        >a.CH4
        >b.CH3COOH
        >c.C2H6;
2 : build>2-methylbutane
    complete>alcohol& 2-propanol >propane;
3 : complete>alcohol >butane;
4 : transform>methane >haloalkane;
```

Figure 4.15: Example of tasks with their specific structure

For some of the tasks it is necessary to present a molecule to the player, and this is an information that is given in the description of the tasks. For this reason, the game needs to have a database with

the molecules that should be loaded in those tasks. The database is a collection of text files, the figure 4.16 is an example of one of these files, each of them corresponds to one molecule, which has several information about the molecule such as: the position it should appear (appears within the two letters 'M'), the different atoms that it has (separated by the letter 'N') and the bonds that exist between the atoms. The bonds each atom has are represented by the ID of the bond and the type that it is, taking the example of the figure 4.16, the Carbon atom has two bonds '_1_2' and '_2_2'. This means the Carbon is connected to the bonds with ID's 1 and 2, and both of those bonds are double, because the second value is 2.

When the task is read, if it has a molecule that should be loaded, it is fetched from the database by its name, and it is loaded into the scene.

```
M(-0.2, 2.0, 0.3)M
N atom: Carbon_4 _(-0.5, 2.0, -0.2)
_1_2
_2_2
N atom: Oxigen_2 _(-0.5, 2.0, -0.1)
_1_2
N atom: Oxigen_2 _(-0.5, 2.0, -0.1)
_2_2
```

Figure 4.16: Example of file used to load a molecule into the scene

Checking challenge completion

Besides those type of files, there are also another type that represent a molecule only through the bonds that it has (figure 4.17). This type of files is used to compare molecules with each other and those files are used to check if the player completed a task correctly, specifically a Complete, Build or Transform task where they have to assemble a specific molecule.

```
Carbon-2-Oxygen
Carbon-2-Oxygen
```

Figure 4.17: Example of file used to compare a molecule to another

The way this comparison is made is through the bonds that the molecule created has, since that is the information that is stored in these files. Because they are text files, the simplest way to compare it with the created molecule, is to have a string with the same information about all the bonds the molecule has. Then the comparison is made between the text file and that string.

There are two phases in comparing the molecules, the first one is to verify that they have the same number of bonds, because if they don't, it means that the molecules don't have the exact same structure and it isn't necessary to check the bonds themselves. The bonds are represented by the atoms it is connecting and the type of bond (simple, double or triple) it is. For this reason, the comparison is

straightforward, if the bond has the same atoms and the same bond type and the bond in the file, then it is considered to be equal. Each bond that exists in the molecule is compared to the bonds represented in the file, and if all of the bonds of the molecule created exist in the file, then the molecule created is the same as the molecule that is represented in the file. This means the molecule created corresponds to the molecule that the task asks the player to create.

The evaluation of the Multiple Choice task is more direct since it is only necessary to check if the answer that the player chose is a match to the correct answer provided in the task description. When the player presses the button that corresponds to the answer he chose, this comparison is performed.

Scoring system

In this phase of development, the two types of scoring of the different tasks were implemented. As in was explained in section 3.1, these types of ranking are Number of Attempts and Number of Moves.

For Number of Attempts the most important part was to correlate the number of answers with the points the player gets. This method is only used with the Multiple Choice tasks, so the point system is specific to this task. The Multiple Choice tasks have 3 possible answers, one is correct and the remaining 2 are wrong, so the points the player can receive from this answer are 3, 2 or 1 points, depending on which attempt he selects the correct answer. This correlation is represented in the figure 4.19.

```
First attempt - 3 points
Second attempt - 2 points
Third attempt and up - 1 point
```

Figure 4.18: Correlation of the number of points the player receives with the number of attempts he makes.

For the Number of Moves, it was necessary to define what should be considered a move, and for this it should take into account the objective of the tasks where the Number of Moves should be applied. Because the tasks that use the Number of Moves are the creating, transforming and completing a molecule, the actions that are counted as moves are bonding two atoms, breaking a bond, picking a new atom, throwing a molecule or an atom to the trash and remove all molecules or all atoms from the scene.

The points the player gets are correlated to the number of moves he makes to solve the task at hand. To get the maximum points, he must solve the task with the minimum moves necessary which depends on the molecule he needs to complete, build or transform and the starting point of the task. For the Complete and Transform task, the starting point is the partial molecule that is placed in front of the player, and for the Build task, the starting point is empty. For this reason, the minimum number of moves is defined at the start of each task, because the value depends on the specifications of the task.

The calculations of the minimum number of moves for each task is tricky because it depends on different aspects: the partial molecule and the asked molecule. It is necessary to check how many

bonds the asked molecule has (which depends on what class it belongs and how many carbons it has) and also how many atoms it has. It is also required to check the same information about the partial molecule, because the minimum number of moves is smaller if the molecule is already partially built.

Due to a tight schedule between the beginning of the final testing phase and the final decision on how to distribute the points for this scoring method, it wasn't possible to fully implement these calculations. They had issues, where the resulting value of minimum moves didn't correspond to the actual value, due to the way the required information is obtained.

The values for the partial molecule are simple to obtain, once it is loaded into the scene, it is only necessary to get the number of children game objects that are present in the parent game object Molecule, because it contains all the atoms and bonds that exist in that molecule. But to get the values of the asked molecule is more difficult, because this information has to be extracted from the details the task itself gives about the molecule. This details can be very explicit which makes it easy to get the needed information. For example, in a Transform task, the details that can be given about the molecule are its class and/or its nomenclature, and if the task is to create a hydrocarbon and its nomenclature is CH4, it is simple to get the information. However, if the task only gives the class, or if the nomenclature is methane, it is trickier to obtain the values necessary to have the minimum number of moves. For this reason, for the final tests the minimum number of moves of each task were hard coded, in order to have both scoring methods tested.

The figure 4.19 shows how the points are given according to the number of moves the player makes to solve the task.

```
Step 1 - # Minimum Number of Moves
Step 2 - # Minimum Number of Moves + 3
Step 3 - # Minimum Number of Moves + 6

# Number of moves = Step 1 - 4 points
Step 2 >= # Number of moves >Step 1 - 3 points
Step 3 >= # Number of moves >Step 2 - 2 points
# Number of moves >Step 3 - 1 point
```

Figure 4.19: Correlation of the number of points the player receives with the number of moves he makes.

Main Menu

One big addition to the game in this stage was the main menu. This was a relatively quick component to add because it used elements that were already used in other scenes, as well as the mechanics.

The player is presented with several boxes of balls (equal to the way the atoms are presented in the game), each of them represents a different game mode: Normal, Speed Run, Tutorial, Build, Complete, Transform and Multiple Choice. To enter one of the modes he must pick up a ball from the box correspondent to the desired mode and place it in the platform that appears in the table in front of him. When
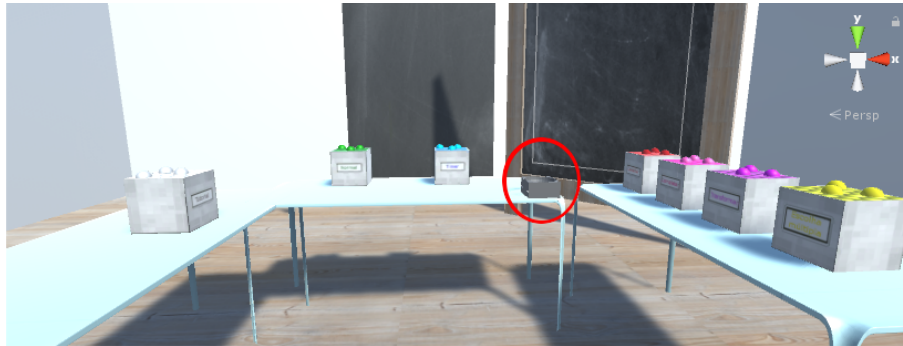
Figure 4.20: Front view of the main menu of the game. The platform used to place the balls is marked with the red circle.

this occurs, the scene correspondent to the game mode is loaded and it begins.

The most important aspect in this component was making sure that the transitions between the several scenes were smooth and quick. This was particularly important because the game is in Virtual Reality and if the transitions are clunky and take too much time, it can create some physical discomfort to the users. However, there weren't big issues when implementing this part since the functions and components that the Unity provides work very well.

Audio and visual feedback

In the first iteration there was already a little visual feedback implemented when a player interacted with the atoms, which was having a thin yellow outline on the atoms when they were grabbed. This was a good start but it wasn't enough, because audio and visual feedback were extremely important to compensate the lack of haptic feedback.

This yellow outline was kept, the only change made to it was to make it thicker so that it was more visible. It was also added an extra outline in red to indicate when the player couldn't connect two atoms together. This red outline appears when a player touches two atoms together where at least one of them doesn't have anymore available bonds to make.

Another good visual aid that was implemented was a representation of the number of bonds that an atom can make. These are represented by small spheres around the atom, and each time the player makes a bond with that atom, the correspondent number of spheres disappears. For example, when making a simple bond, one sphere of each atom disappears, and when making a triple bond, three spheres from each atom disappear.

Lastly, for audio feedback there were different sounds played for different actions. The actions that had audio feedback were: when an atom is grabbed, when the atoms touch each other while the player is grabbing them, when a bond is formed, when a bond is broken, when something is thrown in the trash, and when a button is pressed. The most important sounds are the ones related to manipulating

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the atoms and molecules, because they help the user to have signs of what he is doing.
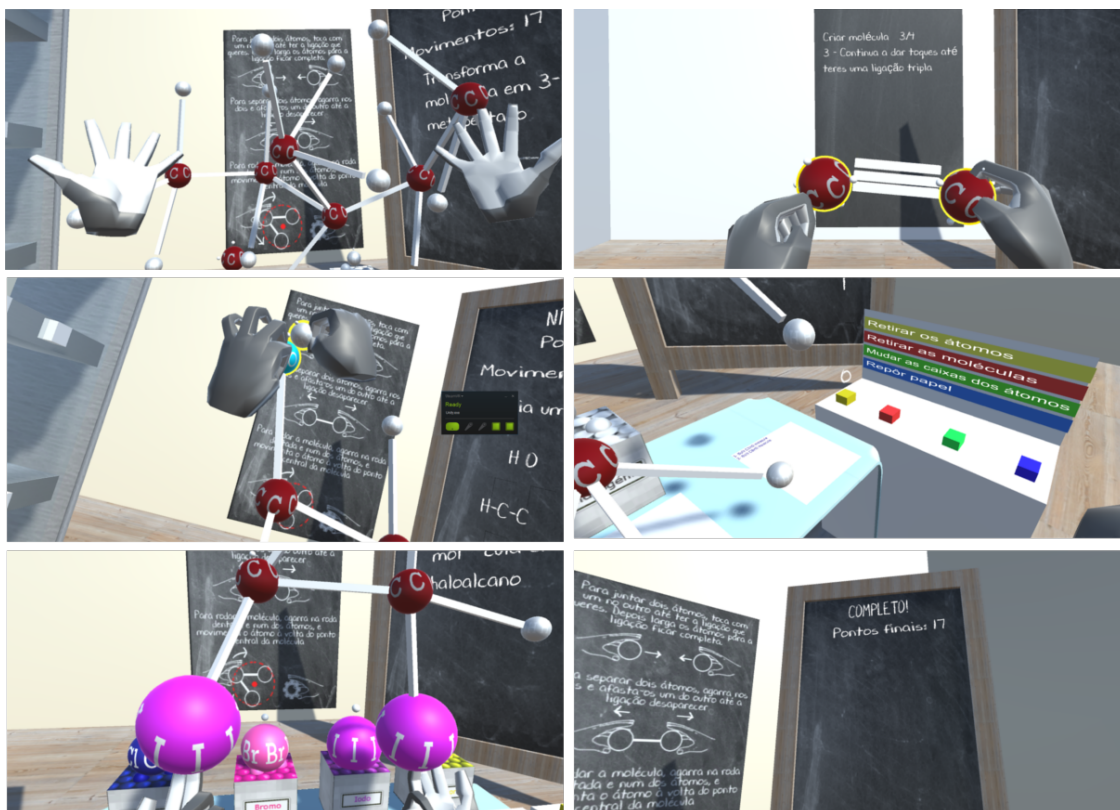

Figure 4.21: Images from the final version of the game

5

Evaluation

Contents

In this chapter the results of the final testing done to the game are going to be presented. This final test had the same structure as the tests performed between the development iterations, where the user was asked to perform a number of tasks and then fill a questionnaire.

In this case, the challenges the user had to perform were to complete the tutorial and also the Normal game mode. As it was detailed in section 3.5, this game mode was thought out to have 50 different levels, but for these tests, it was reduced to 4 levels since it would be extremely time consuming to test 50 levels. The issue with being time consuming will further detailed in this chapter. These 4 levels are a small sample of the first 20 levels, where the focus of each level was a single learning goal. The figure 5.1 details the 4 levels used for testing and the learning goals each tackles. Each level tackles a different learning goal, except level 3 which handles two learning objectives. Ideally there should be 5 levels, however the test was becoming very long and since those two learning goals can be paired together in a single challenge, it was decided to have only 4 levels.

Level 1 (Know the nomenclature of molecules)
    Challenge 1 - Build a CH4 molecule
    Challenge 2 - What is the name of the molecule? (2,2-dimethylbuthane)
Level 2 (Correlate conventional drawings of molecular structures with their 3D structure)
    Challenge 1 - Complete the molecule knowing it's structure (2,2-dimethylbutahne)
    Challenge 2 - Build the molecule from the structure (CH3COOH)
Level 3 (Recognize the functional group a molecule belongs to and knowing the names of functional groups)
    Challenge 1 - Transform the molecule into a haloalkane.
    Challenge 2 - Complete the molecule knowing it is an alcohol
Level 4 (Correlate molecular structure with the nomenclature)
    Challenge 1 - Transform the molecule into a 3-methylpentane.
    Challenge 2 - What molecule is this? (Ethylene)

Figure 5.1: Correspondence of the levels with the learning goals.

The challenges used in the test were shown to the Chemistry teacher Antónia Gomes to make sure that the content of the challenges was correct. The feedback from the teacher was mostly good, although there were some mistakes in one of the Multiple Choice answers, where the nomenclatures of the molecules weren't right.

5.1 Users Sample

This test was performed by high school students at Escola Secundária Raúl Proença in Caldas da Rainha. This was an extremely important aspect because the target audience are high school students and so, the game should be tested by them to get more accurate results regarding the desired population. However, it was only possible to get 8 students to test the game. This was due to three reasons: first the test took at least 30 minutes to perform and the students were leaving mid-class to perform it, so it wasn't possible to have more than 2 students per class; second, it was only possible to have one

student at a time due to the lack of equipment (there was only one HTC Vive and Leap Motion sensor available); and lastly, the students came as volunteers, the test wasn't integrated as part of the class, and for this reason only the interested students showed up to perform it.

The high school students were from the 11th grade and they had Organic Chemistry lessons in the previous school year, which means that they had knowledge about the domain that they had learned recently. Their Chemistry teacher, teacher Antónia Gomes that helped through all the testing process, gave them some revisions on the subjects a week before they performed the tests, so that they wouldn't feel intimidated to do the test. This was important to make them feel comfortable and not worry about knowing everything about the subject, since the objective of the test wasn't to check how knowledgeable they were regarding the domain.

Due to the number of high school students that tested the game is very low, the test was also conducted with students from Instituto Superior Técnico at Campus TagusPark. There were 17 students, ranging between 21 and 28 years old, and they hadn't been in contact with any aspect about Organic Chemistry for several years, so they didn't remember most of the subjects that were approached in the game. For this reason, while they were performing the test, they had a printed sheet available to them with general concepts explained that they needed to know to solve the challenges, in case they needed help to remember something about the subject.

In the following sections, the students from the high school will be referred as Raúl Proença sample and the students from Instituto Superior Técnico will be referred as IST sample.

5.2 Evaluation goals

In order to understand if the game created fulfills its main objective, the results of the tests need to show three different points. One is that the students can easily manipulate the atoms and perform the tasks with ease. Two is that they have fun while they are enhancing their knowledge on Organic Chemistry. And finally three is that the content is accurate to what it is taught in schools.

Another relevant aspect is that the tests should show that the levels can be easily changed by the teachers according to what they want the students to practice.

5.3 Experimental method

On this test, the logging technique was also used to record information concerning each challenge and level posed to the user. The number of moves, the number of attempts and the points that the user made in each challenge since they were the methods used to attribute a score to the user. These values will be compared to the expected values of each challenge to check if there are significant differences.

The questionnaire used was based on the Game Experience Questionnaire (GEQ) [1] and the VR Sickness Questionnaire [2], but it also had 3 more specific questions about the challenges and 2 questions about the scoring methods. The questions about the challenges were made regarding each type of challenge that the user had to tackle: Build, Transform, Complete and Multiple Choice. They asked the user to rank in a linear scale how much did he like to use them, how much fun they were and how interesting. The questions made regarding the scoring methods were made about each one of them, and they asked the users how fair the methods were and how pressured they felt using them.

For this questionnaire it was used the core part of the GEQ, which accesses game experience as scores on seven components: Immersion, Flow, Competence, Positive and Negative Affect, Tension and Challenge. As a robust measure, each component has five items.

It was also used the Post-Game module which assesses how players felts after they had stopped playing. This is relevant to assess naturalistic gaming (when gamers voluntarily decided to play), but it may also be relevant in experimental research. This module has four components, each of them with different number of items attributed to them: Positive Experience (6 items), Negative Experience (6 items), Tiredness (2 items) and Returning to Reality (3 items).

For both modules, the components are evaluated in a linear scale from 1 to 5. For each component of the modules, the average of the items that are attributed to it is calculated, thus obtaining a value that represents each of the components. This process is applied to each user, and then a second average is performed for each component with the values of all the users.
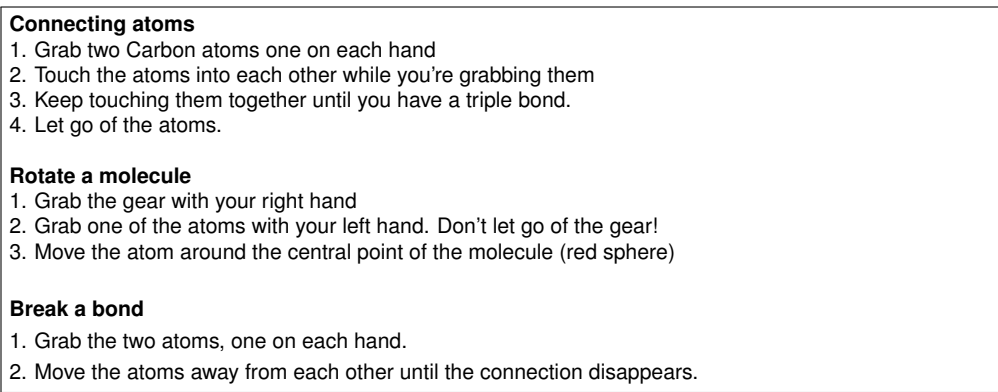
5.4 Results

5.4.1 Tutorial

The tutorial taught the users how to connect two atoms, rotate a molecule and break the connecting, in that order. The steps they had to perform would appear on a blackboard in front of them, and every time they completed one step, it would automatically move on to the next one. The figure 5.2 represents the several steps of the tutorial.

They all completed the tutorial without difficulty, although there were some details that they didn't fully grasped. One of them was how to finalize a connection between two atoms which requires the user to let go both of the atoms. This was most visible right in the first challenge which was to build a methane molecule, which consists of 1 Carbon atom connected to 4 Hydrogen atoms through simple bonds. What happen was that most of the users would grab the Carbon atom and would connect the Hydrogens atoms to it one by one, without ever letting go the Carbon atom. This meant that when

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[1] https://pure.tue.nl/ws/files/21666907/Game_Experience_Questionnaire_English.pdf [accessed: 7/10/2018]
[2] http://w3.uqo.ca/cyberpsy/docs/qaires/ssq/SSQ_va.pdf [accessed: 7/10/2018]

> **Connecting atoms**
> 1. Grab two Carbon atoms one on each hand
> 2. Touch the atoms into each other while you're grabbing them
> 3. Keep touching them together until you have a triple bond.
> 4. Let go of the atoms.
>
> **Rotate a molecule**
> 1. Grab the gear with your right hand
> 2. Grab one of the atoms with your left hand. Don't let go of the gear!
> 3. Move the atom around the central point of the molecule (red sphere)
>
> **Break a bond**
> 1. Grab the two atoms, one on each hand.
> 2. Move the atoms away from each other until the connection disappears.

Figure 5.2: The steps of the tutorial

they finally let go the Carbon atom, it would not have all the bonds created, only the last one he made, because it was the only one the user finalized.

Another aspect that should have been more explicit in the tutorial was how to progress to the next challenge or level, which was through pressing a button that was on the table. During the tutorial they only had to press the button at the end to return to the main menu, so they associated it to return to main menu. When they performed the first challenge, almost all of them asked how they could move on to the next one when they had successfully completed the current task.

5.4.2 Logs

5.4.2.1 Number of moves and number of attempts

The figure 5.3 shows the optimal number of moves and number of attempts for each challenge presented in the test, the average of number of moves and number of attempts performed by the users and their standard deviation. The optimal number of moves corresponds to the minimum number of moves to solve a challenge, and the optimal number of attempts is always one, which means the player chose the correct answer in his first try. The way these values for the optimal number of moves and number of attempts are obtained is described in section 4.1.3.

In the IST sample, the average values for the Multiple Choice challenges are close to the optimal value. Both challenges of this type have a average of 2.39 and 1.33, which are close to the optimal value. In level 1, the interval determined by standard deviation rather large due to an outlier, one of the users made 12 attempts.

The Complete challenge in level 2 had the biggest difference between the optimal value and the average value, where the last one (42.78) is almost double the first one (24). The standard deviation shows that the values vary in a rather large interval around the average value, indicating that the values aren't very consistent and they aren't close to the optimal value.
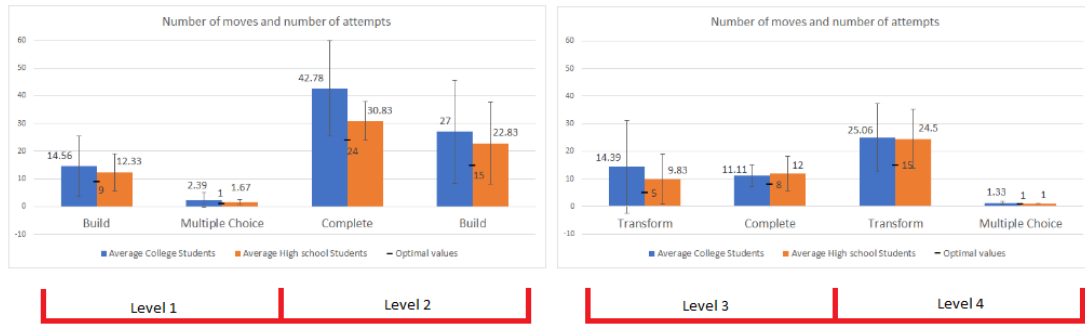
Figure 5.3: Results of number of moves and number of attempts for both samples

The Build challenge in level 2 and both Transform challenges in level 3 and 4 have an average value bigger than the optimal value by around 10 moves. The Transform challenge in level 3 also had an outlier with a value of 78 which caused the standard deviation to translate into a very large interval. According to these averages, their respective standard deviations and intervals, the values are very disperse although their optimal values are encapsulated in those intervals.

Lastly, the Build challenge in level 1 and the Complete challenge in level 3 have the average values closest to their optimal value. However, for the Build challenge, the standard deviation indicates that although the average is close to the optimal value, the values vary in a large interval around the average. For the Complete challenge, on the other hand, the interval defined by the standard deviation indicates that it more likely to have more values close to the average than the Build challenge.

In the Raúl Proença sample, the average values for the Multiple Choice challenges are close to the optimal value, specially the challenge in level 4, which has a standard deviation of 0. This means that all users had the same number of attempts. The challenge on level 1 had very small interval, which indicates that the values are concentrated around the optimal value.

In this sample, there wasn't a standout challenge that displayed a huge difference between the average and the optimal values. These differences are all under 10 moves, and their standard deviations indicate that even though the averages display a difference of 10 moves, the intervals where the values fall are rather big, where the optimal value is included. There are two exceptions, which are the Complete challenge in level 2 and the Transform challenge in level 3. The Transform challenge has an interval, determined by the standard deviation, that is very large, even though it contains the optimal value. This is due to an outlier with a value of 28. The Complete challenge has a small interval around the average of where the values fall, meaning that they are concentrated around the average.

Discussion

From the results of the analyzes of the number of moves and number of attempts, it is possible to say that the high school students had an overall better performance than the students from IST. This

was expected because the high school students had learned Organic Chemistry very recently while the students from IST had not, meaning that they were more prone to make mistakes while trying to solve the challenges and needing to start over.

The expected difficulty in each challenge was fairly close to the actual difficulty displayed by the users. However, there were some challenges were issues with the implementation caused big disparities that could have been much lower had those problems not existed. The results from the Complete challenge from level 2 are an example of the effect of those issues. The problem was that the implementation didn't take into account the situation where a player would try and connect two molecules into one. And because the implementation couldn't handle that case, when the users tried to join two molecules, it caused problems in checking if the molecule was correct or not, because the code didn't recognize it as one unique molecule. For this reason, the users were forced to restart the molecule, being careful not to join two molecules, and thus making a lot more moves than what was expected.

5.4.2.2 Scores

The figure 5.4 presents the averages of the points the users received in each challenge.

The average values in the IST sample are all very close to each other in every challenge, while in the Raúl Proença sample there is some variation in the average values. The Multiple Choice challenges have the highest averages, in both samples, considering the maximum value possible is 3. Overall, the Raúl Proença sample has higher averages than the IST sample, but this could be influenced by the number of users each sample has.

The challenge where the difference between the two samples is more notorious is in the Transform challenge in level 3, where the IST average is 2.22 and the Raúl Proença average is 3.17. Their standard deviations are similar, but because the average value is not close, it translates to different intervals. This indicates that the points the users from the IST sample received varies more than the points the users from the Raúl Proença sample received.

The Complete challenge from level 2 also has a big difference between both samples, the IST average is 1.44 and the Raúl Proença average is 2.33. But because their standard deviations have similar values (proportionally to their averages), it means that both samples have a similar range in which their values can fall.

Discussion

From the analyzes of the points received, it is possible to say that some challenges were more difficult to solve than what it was expected. Even though there were some issues cause by the implementation of the mechanics, the users that weren't affected by these problems, still needed more moves to accurately solve the challenge than what it was predicted. This is particularly noticeable in the Complete

Level 1					
Build			Multiple Choice		
Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$	Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$
4	2.94 ± 1.21	3 ± 1.09	3	2.33 ± 0.97	2.33 ± 0.82

Level 2					
Complete			Build		
Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$	Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$
4	1.44 ± 0.86	2.33 ± 1.21	4	2.28 ± 1.27	2.5 ± 1.22

Level 3					
Transform			Complete		
Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$	Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$
4	2.22 ± 1.35	3.17 ± 1.17	4	2.78 ± 1.11	3 ± 1.55

Level 4					
Transform			Multiple Choice		
Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$	Max	IST Average $\pm\ \sigma$	Raúl Proença Average$\pm\ \sigma$
4	2 ± 1.03	2.17 ± 0.98	3	2.61 ± 0.61	3 ± 0

Figure 5.4: Average of points the users received on each challenge

challenge from level 2 and the Transform challenge in level 4, in which users from both samples received lower points comparing to the points received in the other challenges. These questions were already considered has the most difficult out of all challenges, but the results showed that they were even more difficult then expect. For the IST sample, one of the reasons for this difference in difficulty can come from lack of knowledge about the domain, since these particular challenges are more though to answer if the user doesn't know a considerate amount of information about the subjects.

The remaining challenges were easier to solve and the points received on them were within the expected values for both samples. As predicted, overall the high school students have higher average values than the students of IST, due to their knowledge on Organic Chemistry being more recent, although these values could change had the number of users been equal for both samples.

5.4.3 Game Experience

As it was mentioned in section 5.3, this questionnaire had the core and Post-Game modules from the GEQ. The figure 5.5 details the results from both core and post-game modules, and the figure 5.6 shows the results from the T-Test comparison between samples for each component of the modules.

Although the averages of each component seem to be fairly similar between the two samples, after performing the T-test comparing the values of all users of the two samples, is shows that only the Negative Affect component doesn't have a significant difference.

In both samples, it is possible to see that the Negative Affect and Tension have the lowest results while the Positive Affect, Flow and Immersion have the highest values. This means that the users had a overall positive experience while playing the game, they felt immersed in it and that it had flow, meaning
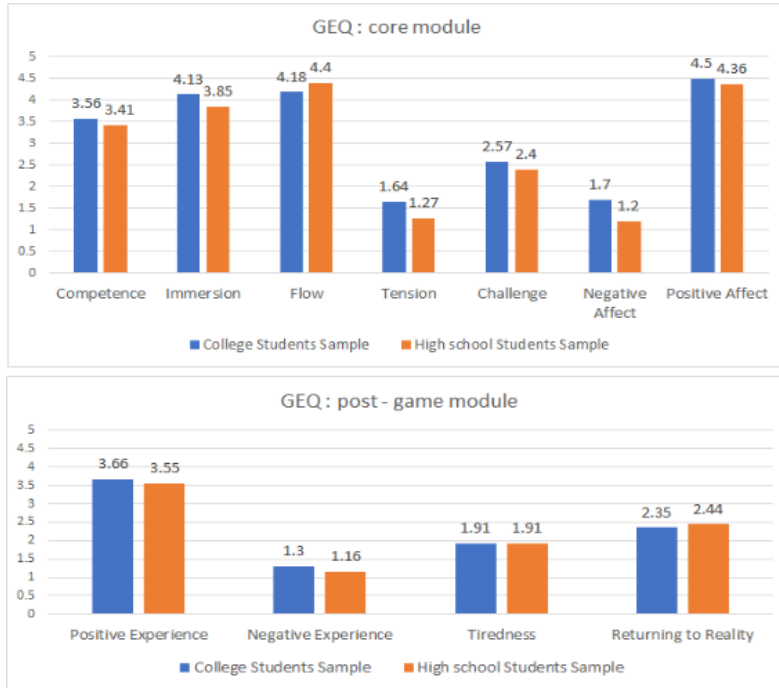
Figure 5.5: GEQ section: Core and Post-Game module results

Post-Game components	Positive Experience		Negative Experience		Tiredness		Returning to Reality	
T-Test (p value)	0.3886		0.2384		0.4954		0.4315	
Core components	Competence	Immersion	Flow	Tension	Challenge	Negative Affect		Positive Affect
T-Test (p value)	0.3677	0.1185	0.2565	0.1078	0.3370	0.0192		0.2946

Figure 5.6: GEQ Section: T-Test comparison between both samples for each module

that they knew what they should do during the test and didn't get stuck. The Competence component has a slightly lower value comparing to the components with the highest values, they are 3.56 and 3.41. This means that the users felt competent while playing the game, but not too much. The Challenge component has a even lower values than the Competence component, which are 2.57 and 2.4, which is interpreted as they didn't really feel challenged by the game.

Much like the results from the core module, the averages between both samples from the post-game module have very close values, and the T-Test performed reveals that they don't have significant differences, except in the negative affect component.

For both samples, the Negative Experience and the Tiredness components have the lowest values. This means that overall the users didn't have a negative experience with the game and that they didn't feel too tired at the end of the testing session. The Positive Experience had the highest value, although it wasn't extremely high, which means that the users had a fairly positive experience with the game. The Returning to Reality component had medium values of 2.35 and 2.44, which indicates that the users had a little bit of a difficult time adjusting to reality after the session, but it wasn't too hard.

Discussion

From the analyzes of the section of the questionnaire about Game Experience, the conclusions are that overall the users had a positive experience with the game. They felt immersed in it and they felt skillful while playing it, which is heavily related with the mechanics of manipulation. This can indicate that the mechanics they used help in making the users feel competent. Another important aspect is the game flow, which had high values, meaning that the users felt that the game had a smooth progression. This could have been an issue for users who had less knowledge on Organic Chemistry, but because they had information available to them that they could consult, they didn't get lost in any step of the game.

The Challenge aspect of the game had the lowest scores which isn't necessarily a bad sign. These values aren't surprising because the challenges are based on Organic Chemistry and they aren't very complex, which means that anyone with a basic to moderate level of knowledge on this subject can easily solve the challenges. Given that the high school students had had revisions on the domain prior to the test, and that the students from IST had information about the subject available to them, it is reasonable that the game wasn't considered extremely challenging.

The Post-Game module results also indicate that the overall experience was positive, with little negative aspects and tiredness from the users. This could have been an issue given that the users spent most of the time with their arms up and moving the around to interact with the atoms and the molecules.

The values between both samples were compared to understand if the experience is different depending on the audience it is presented to. Given that there was only one component that had no significant difference, it means that it does have some impact. However, even though there are significant differences between the several components, the results individually were still good.
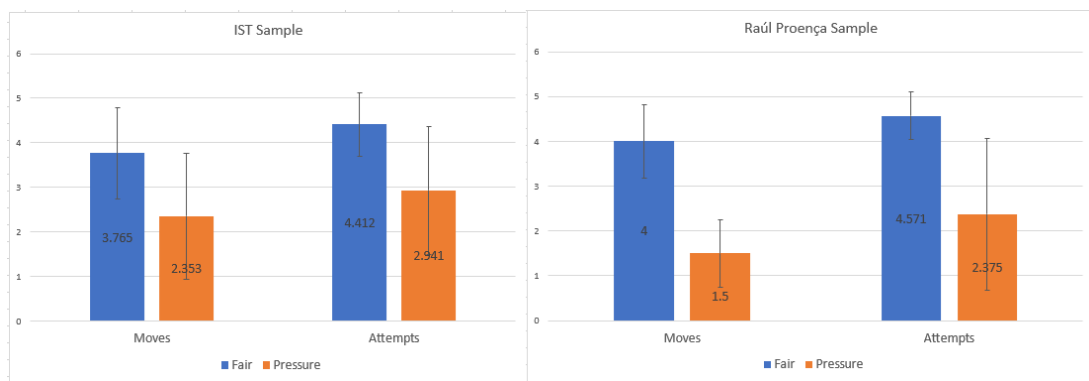
5.4.3.1 Specific Questions

The figure 5.7 depicts the results from the specific questions about the different challenges, and the figure 5.8 details the results regarding the scoring methods.

In both samples, the challenges had high averages and the intervals determined by their standard deviations show that the values are concentrated around their average value. In the IST sample, the Multiple Choice challenge has the lowest averages for all aspects, even though they are still above the average of 2.5 (considering that the maximum value is 5). The standard deviations for this challenge are higher, translating into a bigger interval, indicating that the values are more scattered.

In both samples, the scoring methods had high averages for fairness, although in the IST sample, the interval determined by the standard deviation, regarding the fairness of the Number of Moves method is bigger than the others. This shows that the values are more disperse for this particular case. The average for pressure felt vary more between samples and they have big values for standard deviations,
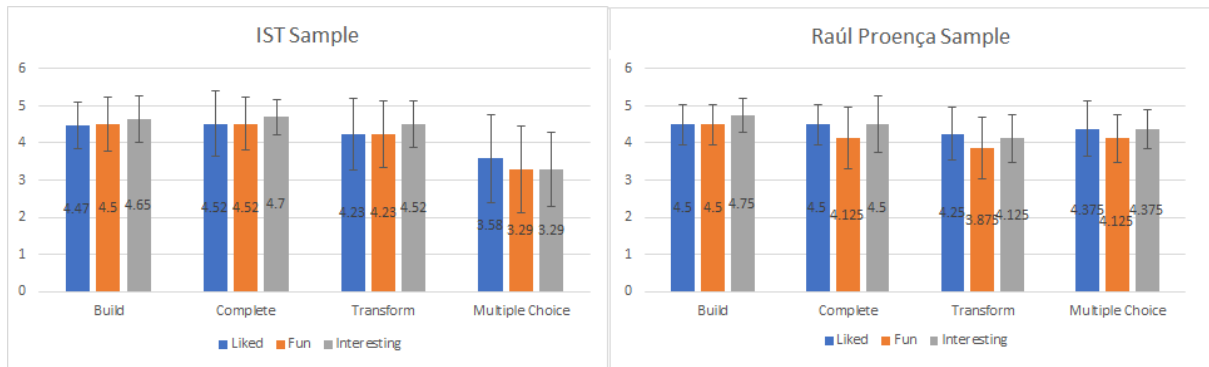
Figure 5.7: Results from the specific questions about the challenges.

Figure 5.8: Results from the specific questions about the scoring methods.

which translates into large intervals where the values concentrate. This means that the values chosen for evaluating the pressure felt are very disperse.

Discussion

From the analyzes of the results from the specific questions about the challenges and the scoring methods, the conclusions are that overall the users liked all types of challenge. Even though the Multiple Choice challenge was the least liked and considered the least fun and least interesting by the users from the IST sample, it still had high average values.

Regarding the scoring intervals, the users found the scoring methods to be fair and felt more pressure with the Number of Attempts than the Number of Moves. However, since the values are very dispersed, it isn't possible to say if they cause a lot of pressure or not.

However, all the results could be very different if the samples had the same number of users.

5.4.3.2   VR Sickness

The VR Sickness assesses two components which are nausea and oculo-motor. The figure presents the results for this section of the questionnaire.
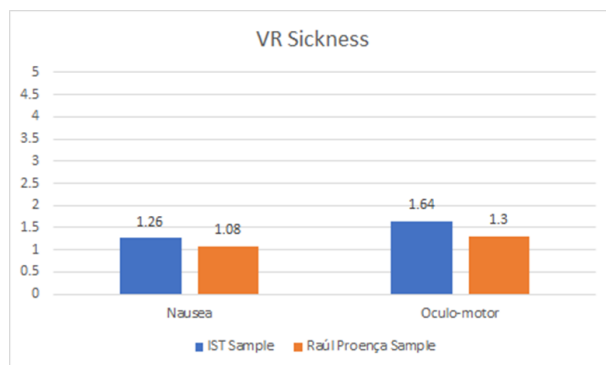
	Nausea	Oculo-motor
T-Test	0.1018	0.0606

Figure 5.9: Results from the VR Sickness section.

In similarity to the other sections of the questionnaire, the average values for the Nausea and Oculo-motor components are very close, but they still have a significant difference between them, as it is shown by the T-Test.

Despite that, it is possible to see that, for both samples, the users felt almost no nausea and had no issues with their vision or motor skills after they finished the test.

5.4.4 Observations

During the tests on both samples there were some observations made, mainly to understand if the users were having fun or feeling frustrated or annoyed.

All the high school students had fun while playing the game, some of them even said it at the end of the test. Even the users who faced some difficulties during the test, due to problems in the implementation, still enjoyed playing the game. They also seemed focused on solving the challenges and were concentrating on finding out the answer without any help.

Most of the users from the IST sample had fun and enjoyed playing the game. About 5 of all the users were quiet and not very expressive during the test, although the results from the questionnaire don't show discontent or negative experiences with the game. From the 17 users, 9 of them were really focusing and trying to find out the correct answer by themselves without any help, except from the information that they had available to them. Half of the users mentioned at the end of the test that the game made them re-learn what they knew about Organic Chemistry, and that it was more fun to learn about this subject through this game rather than the traditional method.

5.4.5 Interview to a Chemistry teacher

In order to have the point of view of a chemistry teacher, an interview was made to the teacher Antónia Gomes. The teacher not only saw the some students playing but also played the game at the end of the testing phase in the high school. This questionnaire was made via email and is going to be translated from Portuguese to English. The original one can be seen in the appendix B.

How reliable is the representation of the molecules and atoms comparing to the representations used in books and in traditional models?

Answer: The representation of the molecule is well made.

Are the challenges presented in the game faithful to the style of exercises that exist in books?

Answer: Yes, they correspond to the exercises that students are asked to solve.

What advantages and disadvantages the game has comparing to the traditional teaching methods on Organic Chemistry?

Answer: It's more appealing to solve the exercises through the game than through paper and pencil, however it requires more time to solve them.

How would you use the game in a class about Organic Chemistry?

Answer: In a classroom, it is possible to have 30 students simultaneously. If the game is used in a laboratory class, there can be 15 students at maximum. We would have to have the necessary equipment to have all those students playing the game at the same time. If the schools has a room with all the required equipment, it makes the process easier.

Does the game help to approach Organic Chemistry in a more entertaining way?

Answer: Yes. Without a doubt, it is a good method to cement the knowledge in a fun way.

5.4.5.1 Discussion

By analyzing the answers given by the teacher, the game might be a good tool to be used in the classroom to help teach Organic Chemistry. It would require to have more equipment available at the school to have several students play it at the same time, but it might be able to bring fun and entertainment in learning the subject.

6

Conclusion

Contents

At the start, the domain of the game was presented in a broad and general view, where the basic knowledge of Organic Chemistry were presented. However, since the target audience are high school students, the domain was restricted to the main subjects that the students learn about the domain in high school. As a result, the game has 5 learning objectives that it must help the students to learn and improve.

After analyzing different games and applications, some of them are featured for their qualities but also for what it didn't work in them. These games and applications were very helpful to have a base of "do's and don't's" regarding Virtual Reality, educational games and games about Organic Chemistry. The game had three development iterations and each of them had a testing phase to check if the implementation on that stage was having the expected results or not.

6.1 Results

The most important achievement present in this work is the creation of a functional educational game which is fun and entertaining to play. Although it was only implemented a small version of the Normal game mode, all the proposed mechanics in the concept were implemented as well as the most crucial audio and visual feedback. The levels and the different challenges were implemented as they were thought out with the additional flexibility, which wasn't tested with users, but it enables them to change the challenges as they see fit. This would be used by the teachers, so that they could change the levels and challenges according to what they were teaching in each class.

The results obtained were overall very good. All the users enjoyed playing the game, even the ones that didn't have as much knowledge about Organic Chemistry as the high school students. It was visible the potential the game as in a class room environment and the impact in learning Organic Chemistry, particularly in those users with little knowledge. The need to solve the challenges correctly and gain the maximum number of points made them invested in learning the concepts needed by themselves and understand about the domain. In the case for the high school students, it was possible to see that they were applying the knowledge that they already had, and when they made a mistake, they analyzed why it was wrong and were able to understand how to correct it and solve it. Even though there were problems during the tests, the users still felt comfortable with the mechanics and they didn't have difficulties in understanding how to manipulate the molecules and atoms.

6.2 Problems and difficulties

In the development of the game, there were some challenges and difficulties. One of the major difficulties was the implementation of the rotation of molecules, because it was the hardest type of ma-

nipulation to implement in the most natural and intuitive way possible. In the first iteration of development, there were three different methods thought out and implemented, which were tested at the end of this first stage. Due to complications with the logs and obtaining sufficient data to reach a decisive conclusion, the implementation of the rotation was a big focus on the second iteration. It was only after this second stage of development and the respective testing phase, that the method of rotation was officially set.

Another issue that only surfaced in the final tests and that brought significant problems during the tests, was that the connecting of two molecules wasn't implemented. The players could only join two atoms together, or an atom to an existing molecule, but they could not connect two molecules together. This wasn't caught on early stages because the tests regarding the connection of atoms and molecules didn't have this situation, and during the development stage this case never came up.

One aspect that was planned on being tested was the teachers being able to customize the levels as they wished. The implementation is prepared to handle this, because the levels aren't hard coded, they are read from a text file with a specific structure that can be altered. However, these text files aren't user friendly and it would have been difficult for someone who isn't familiar with how the code handles the text file to make a mistake and the levels wouldn't be loaded correctly. For this reason, these component wasn't tested.

Finally, it was rather challenging to perform the tests in the Escola Secundária Raúl Proença due to several reasons. The first was setting dates to be there performing the tests without compromising their class time and that it wasn't too close to the deadline of this thesis. Their classes started in the third week of September, and it was only possible to perform the tests on one day of the final week of September. The second was having only one HTC Vive and one Leap Motion sensor available to perform the tests, which meant that it wasn't possible to have more than one user testing at a time. The third and final reason was that the students came at their own will, which meant that only the interested students would come and perform the tests. The bad thing about this is that it meant that the number of students that would participate wasn't certain, because it depended on their will, interest and free time. Had it been planned to have the testing integrated in a class, it would have been easier to have more students performing the test.

6.3 Future Work

The first point that should be tackle in future work is implement the possibility to join two molecules together, because not being able to do this is a major flaw in the game, and it takes away a bit of freedom on how the players can interact with molecules. The second point would be to fully implement all the game modes that were present in the final concept of the game. This would make it more interesting and

add more potential as a tool to be used in the classroom, considering that it has not only two generic modes (Normal and Speed Run) but it also as specific modes for the different types of challenges available. The third and final point would be to implement a tool that would enable the teachers to design and create the levels for the game with a user friendly interface, and it would automatically create all the necessary text files for the game to load the levels correctly. This would be very beneficial because they could customize the game at their own will, according to what they want or need their students to learn at a specific class. The game would become more flexible and dynamic to be used in the classrooms.

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A

Questionnaires

A.1 First Iteration Questionnaire

Questionário

Este questionário tem por objectivo avaliar o protótipo das mecânicas de um jogo para ensinar Química Orgânica. Este jogo será desenvolvido no âmbito da cadeira de Dissertação, no Mestrado de Engenharia Informática e de Computadores.

* Required

Informação

1. **Género:** *
   Mark only one oval.

   ( ) Masculino

   ( ) Feminino

2. **Idade:**
   Mark only one oval.

   ( ) 18 - 21

   ( ) 22 - 25

   ( ) 26 - 29

   ( ) 30 -

3. **Já teve contacto com alguma tecnologia de Realidade Virtual?** *
   Mark only one oval.

   ( ) Sim

   ( ) Não

4. **Se sim, indique qual a tecnologia e qual a aplicação da mesma (jogo, simulação, vídeo, entre outros)**

   _____

   _____

   _____

   _____

   _____

Rotação de moléculas

Para ajudar na resposta às seguintes perguntas estão aqui descritos os diferentes métodos que testou:

Método 1 - Automático
Método 2 - Mão Livre
Método 3 - Pivot

5. **Ordene por ordem crescente, os diferentes métodos de rotação de acordo com o seu nível de complexidade**

   _____

6. **Ordene, por ordem crescente, os diferentes métodos de rotação de acordo com quão intuitivos são.**

   _____

7. **Ordene, por ordem crescente, os diferentes métodos de rotação de acordo com a facilidade de utilização.**

   _____

8. **Para os métodos 1 e 2 (Automático e Mão Livre), indique qual o modo mais fácil de definir o eixo de rotação.**
   Mark only one oval.

   - ( ) Palma para cima e palma para baixo
   - ( ) Palma para o lado e palma para o corpo

9. **Para o método 1 (Automático), indique qual o modo mais fácil de definir o eixo de rotação.**
   Mark only one oval.

   - ( ) Palma para cima e palma para baixo
   - ( ) Palma para o lado e palma para o corpo

10. **Para o método 1 (Automático), indique qual o modo mais intuitivo de definir o eixo de rotação.**
    Mark only one oval.

    - ( ) Palma para cima e palma para baixo
    - ( ) Palma para o lado e palma para o corpo

11. **Para o método 2 (Mão Livre), indique qual o modo mais fácil de definir o eixo de rotação.**
    Mark only one oval.

    - ( ) Palma para cima e palma para baixo
    - ( ) Palma para o lado e palma para o corpo

12. **Para o método 2 (Mão Livre), indique qual o modo mais intuitivo de definir o eixo de rotação.**
    Mark only one oval.

    - ( ) Palma para cima e palma para baixo
    - ( ) Palma para o lado e palma para o corpo

13. **Qual dos diferentes métodos preferiu utilizar? Porquê?**

_____

_____

_____

_____

_____

Movimentação

Para ajudar na resposta às seguintes perguntas estão aqui descritos os diferentes métodos que testou:

Método 1 - Pivot
Método 2 - Atómos

14. **Indique qual o método mais intuitivo.**
Mark only one oval.

  ◯ Método 1 - Pivot

  ◯ Método 2 - Átomos

15. **Indique qual o método mais fácil de utilizar.**
Mark only one oval.

  ◯ Método 1 - Pivot

  ◯ Método 2 - Átomos

16. **Indique qual o método mais complexo.**
Mark only one oval.

  ◯ Método 1 - Pivot

  ◯ Método 2 - Átomos

17. **Indique qual o método que preferia utilizar.**
Mark only one oval.

  ◯ Método 1 - Pivot

  ◯ Método 2 - Átomos

Ligações de moléculas

Para ajudar na resposta às seguintes perguntas estão aqui descritos os diferentes métodos que testou:

Método 1 - Distância
Método 2 - Taps

18. **Indique qual o método mais fácil de utilizar.**
Mark only one oval.

  ◯ Método 1 (Distância)

  ◯ Método 2 (Taps)

19. **Indique qual o método mais intuitivo.**
Mark only one oval.

◯ Método 1 (Distância)

◯ Método 2 (Taps)

20. **Indique qual o método mais complexo.**
Mark only one oval.

◯ Método 1 (Distância)

◯ Método 2 (Taps)

21. **Indique qual o método que preferia utilizar.**
Mark only one oval.

◯ Método 1 (Distância)

◯ Método 2 (Taps)

VR Sickness

22. **Indique o seu nível de desconforto ao longo da sessão.**
Mark only one oval.

	1	2	3	4	5	
Pouco	◯	◯	◯	◯	◯	Muito

23. **Indique o seu nível de fatiga após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	◯	◯	◯	◯	◯	Muito

24. **Indique dos sintomas abaixo, quais está a sentir neste momento.**
Check all that apply.

☐ Dor de cabeça

☐ Dificuldade em focar a vista

☐ Tonturas

☐ Enjoos

A.2 Second Iteration Questionnaire

Questionário

Este questionário tem por objectivo avaliar as mecânicas de interação de um jogo para ensinar Química Orgânica. Este jogo será desenvolvido no âmbito da cadeira de Dissertação, no Mestrado de Engenharia Informática e de Computadores.

* Required

Informação

1. **Género: ***
   Mark only one oval.

   ⃝ Masculino

   ⃝ Feminino

2. **Idade:**
   Mark only one oval.

   ⃝ 18 - 21

   ⃝ 22 - 25

   ⃝ 26 - 29

   ⃝ 30 -

3. **Já teve contacto com alguma tecnologia de Realidade Virtual? ***
   Mark only one oval.

   ⃝ Sim

   ⃝ Não

4. **Se sim, indique qual a tecnologia e qual a aplicação da mesma (jogo, simulação, vídeo, entre outros)**

   _____

   _____

   _____

   _____

   _____

5. **Participou em algum teste anterior relativo a este projecto? ***
   Mark only one oval.

   ⃝ Sim

   ⃝ Não

Rotação de moléculas

Para ajudar na resposta às seguintes perguntas estão aqui descritos os diferentes métodos que testou:

Método A - Pulso (roda a molécula através da rotação do pulso)
Método B - Pivot (roda a molécula através da rotação de um átomo em torno do ponto central da molécula)

6. **Indique o nível de facilidade de utilização do método A (Pulso)**
   Mark only one oval.

	1	2	3	4	5	
Fácil	◯	◯	◯	◯	◯	Díficil

7. **Indique o nível de facilidade de utilização do método B (Pivot)**
   Mark only one oval.

	1	2	3	4	5	
Fácil	◯	◯	◯	◯	◯	Díficil

8. **Indique o nível de compreensão do funcionamento do método A (Pulso) na primeira utilização.**
   Mark only one oval.

	1	2	3	4	5	
Fácil de perceber	◯	◯	◯	◯	◯	Díficil de perceber

9. **Indique o nível de compreensão do funcionamento do método B (Pivot) na primeira utilização.**
   Mark only one oval.

	1	2	3	4	5	
Fácil de perceber	◯	◯	◯	◯	◯	Díficil de perceber

10. **Indique o nível de precisão que teve ao realizar as tarefas com o método A (Pulso)**
    Mark only one oval.

	1	2	3	4	5	
Pouca	◯	◯	◯	◯	◯	Muita

11. **Indique o nível de precisão que teve ao realizar as tarefas com o método B (Pivot)**
    Mark only one oval.

	1	2	3	4	5	
Pouca	◯	◯	◯	◯	◯	Muita

12. **Qual dos dois métodos preferiu utilizar?**
Mark only one oval.

⬭ Método A (pulso)

⬭ Método B (pivot)

13. **Porquê?**

_____

Skip to question 14.

VR Sickness

14. **Indique o seu nível de desconforto ao longo da sessão.**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

15. **Indique o seu nível de fatiga após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

16. **Indique o seu nível de tonturas com os olhos abertos após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

17. **Indique o seu nível de tonturas com os olhos fechados após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

18. **Indique o seu nível de visão desfocada após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

19. **Indique o seu nível de enjoo após a sessão**
Mark only one oval.

	1	2	3	4	5	
Pouco	⬭	⬭	⬭	⬭	⬭	Muito

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A.3 Final test Questionnaire

Questionário

Este questionário tem por objectivo avaliar o gameplay de um jogo para ensinar Química Orgânica. Este jogo será desenvolvido no âmbito da cadeira de Dissertação, no Mestrado de Engenharia Informática e de Computadores.

* Required

Informação geral

1. **Género:** *
   Mark only one oval.

   ◯ Masculino

   ◯ Feminino

2. **Idade:**
   Mark only one oval.

   ◯ 15 - 18

   ◯ 19 - 22

   ◯ 23 - 26

   ◯ 27 - 30

   ◯ 31 -

3. **Já teve contacto com alguma tecnologia de Realidade Virtual?** *
   Mark only one oval.

   ◯ Sim

   ◯ Não

4. **Se sim, indique qual a tecnologia que utilizou (HTC Vive, Playstation VR, entre outros) e qual a aplicação (jogo, simulação, vídeo, entre outros)**

   _____

5. **Participou em algum teste anterior relativo a este projecto?** *
   Mark only one oval.

   ◯ Sim

   ◯ Não

Desafios

As perguntas seguintes serão sobre os desafios que foram colocados ao longo do jogo.

6. **Indica na escala, quanto gostaste dos desafios de construir moléculas**
   Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

7. **Indica na escala, quanto gostaste dos desafios de completar moléculas**
   Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

8. **Indica na escala, quanto gostaste dos desafios de transformar as moléculas**
   Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

9. **Indica na escala, quanto gostaste dos desafios de escolha múltipla**
   Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

10. **Indica na escala, quão divertidos são os desafios de construir moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

11. **Indica na escala, quão divertidos são os desafios de completar moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

12. **Indica na escala, quão divertidos são os desafios de transformar as moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

13. **Indica na escala, quão divertidos são os desafios de escolha múltipla**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

14. **Indica na escala, quão interessantes são os desafios de construir moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

15. **Indica na escala, quão interessantes são os desafios de completar moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

16. **Indica na escala, quão interessantes são os desafios de transformar as moléculas**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

17. **Indica na escala, quão interessantes são os desafios de escolha múltipla**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

Pontuação

As perguntas seguintes serão sobre a pontuação que foi utilizada ao longo do jogo.

18. **Indica na escala, quão pressionado(a) te sentiste a ser pontuado pelo número de movimentos que fazias.**
    Mark only one oval.

	1	2	3	4	5	
Nada	◯	◯	◯	◯	◯	Bastante

19. **Indica na escala, quão justo sentiste que a pontuação era utilizando o número de movimentos que fazias.**

Mark only one oval.

	1	2	3	4	5	
Nada	⬭	⬭	⬭	⬭	⬭	Bastante

20. **Indica na escala, quão pressionado(a) te sentiste a ser pontuado pelas tentativas de resposta que davas nas tarefas de Escolha Múltipla.**

Mark only one oval.

	1	2	3	4	5	
Nada	⬭	⬭	⬭	⬭	⬭	Bastante

21. **Indica na escala, quão justo sentiste que a pontuação era utilizando as tentativas de resposta que davas nas tarefas de Escolha Múltipla.**

Mark only one oval.

	1	2	3	4	5	
Nada	⬭	⬭	⬭	⬭	⬭	Bastante

22. **Qual foi o modo de pontuação que gostaste mais?**

Mark only one oval.

⬭ Número de movimentos

⬭ Número de tentativas de resposta

Game experience - durante o jogo

Para cada pergunta, indica como te sentiste durante o jogo tendo em conta a escala utilizada.

23. **Senti-me contente.**

Mark only one oval.

	1	2	3	4	5	
Não de todo	⬭	⬭	⬭	⬭	⬭	Extremamente

24. **Senti-me hábil.**

Mark only one oval.

	1	2	3	4	5	
Não de todo	⬭	⬭	⬭	⬭	⬭	Extremamente

25. **Estava interessado(a) na história do jogo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

26. **Eu achei-o divertido.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

27. **Estava totalmente ocupado(a) com o jogo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

28. **Senti-me feliz.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

29. **Fiquei de mau humor.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

30. **Pensei noutras coisas.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

31. **Achei-o cansativo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

32. **Senti-me competente**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

33. **Achei-o difícil.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

34. **Achei que era esteticamente agradável.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

35. **Esqueci-me de tudo à minha volta.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

36. **Senti-me bem.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

37. **Era bom a jogá-lo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

38. **Senti-me aborrecido(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

39. **Senti que tive sucesso.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

40. **Senti-me imaginativo(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

41. **Senti que podia explorar.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

42. **Gostei do jogo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

43. **Era rápido(a) a atingir os objectivos do jogo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

44. **Senti-me chateado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

45. **Senti-me pressionado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

46. **Senti-me irritado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

47. **Perdi a noção do tempo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

48. **Senti-me desafiado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

49. **O jogo impressionou-me.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

50. **Estava completamente concentrado(a) no jogo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

51. **Senti-me frustrado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

52. **Senti que foi uma experiência enriquecedora.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

53. **Perdi ligação com o mundo exterior.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

54. **Senti pressão de tempo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

55. **Tive de me esforçar bastante.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

Game experience - após o jogo
Para cada pergunta, indica como te sentiste após teres jogado, tendo em conta a escala utilizada.

56. **Senti-me revigorado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

57. **Senti-me mal.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

58. **Senti que foi difícil voltar à realidade.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

59. **Senti-me culpado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

60. **Senti que foi uma vitória.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

61. **Achei que foi uma perda de tempo.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

62. **Senti-me com energia.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

63. **Senti-me satisfeito(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

64. **Senti-me desorientado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

65. **Senti-me exausto(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	◯	◯	◯	◯	◯	Extremamente

66. **Senti que podia ter estado a fazer coisas mais úteis.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

67. **Senti-me poderoso(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

68. **Senti-me inquieto(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

69. **Senti-me arrependido(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

70. **Senti-me envergonhado(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

71. **Senti-me orgulhoso(a).**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

72. **Tive a sensação que tinha voltado de uma aventura.**
Mark only one oval.

	1	2	3	4	5	
Não de todo	○	○	○	○	○	Extremamente

VR Sickness

Indique quanto cada sintoma te está a afectar neste momento.

73. **Desconforto geral**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

74. **Fatiga**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

75. **Dor de cabeça**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

76. **Vista em esforço**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

77. **Dificuldade em focar**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

78. **Suor**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

79. **Náuseas**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

80. **Dificuldade em concentrar**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

81. **Visão desfocada**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

82. **Tonturas de olhos abertos**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

83. **Tonturas de olhos fechados**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

84. **Vertigo (sensação de vertigens)**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

85. **Desconforto no estômago**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

86. **Vontade de arrotar**
Mark only one oval.

	1	2	3	4	5	
Nenhum	◯	◯	◯	◯	◯	Severo

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A.4   Teacher Questionnaire

- Quão fidedigna é a representação das moléculas e átomos em relação às representações utilizadas nos livros e em modelos tradicionais?

  R: A representação das moléculas está bem feita.

- Os desafios apresentados no jogo são fiéis ao estilo de exercícios que existem nos manuais?

  R: Sim, correspondem aos exercícios solicitados aos alunos.

- Que vantagens e desvantagens o jogo traz em relação aos métodos tradicionais de ensino de Química Orgânica?

  R: É mais aliciante do que resolver exercícios com papel e lápis, no entanto, requer muito mais tempo para fazer os mesmos exercícios.

- Como aplicaria o jogo no contexto de uma aula sobre Química Orgânica?

  R: Numa sala de aula, podemos ter, em simultâneo, 30 alunos. Se for aplicado numa aula de turno, teremos no máximo 15 alunos. Teríamos que ter o equipamento necessário para que estes alunos estivessem a jogar em simultâneo. Se na escola houver uma sala com estes equipamentos, torna-se fácil.

- O jogo ajuda a abordar a Química Orgânica de um modo mais divertido?

  R: Sim. Sem dúvida, é uma boa maneira de consolidar os conhecimentos de forma divertida.