Virtual Reality Game to teach Organic Chemistry

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Abstract. This paper describes the work conducted to develop a game in Virtual Reality to help teach Organic Chemistry. Other educational games were analysed to identify their strengths and weaknesses and the importance of games and Virtual Reality technologies in education were studied to obtain guidelines on how to approach the implementation of this game. The manipulation of objects was also studied because it is extremely important in Virtual Reality and it takes a central focus in this game because the player will be manipulating atoms and molecules. To help with this component, the Leap Motion sensor was used alongside the HTC Vive. The game development, which includes mechanics and gameplay, was done in three iterations. There was an evaluation performed per iteration, and a final evaluation was performed at the last iteration with high school students. The results showed that the approach of using VR is viable for teaching Organic Chemistry.

Keywords: Virtual Reality, Organic Chemistry, Serious Games, Gestural Interfaces

1 Introduction

This paper describes the development of a game to improve and complement the traditional methods of teaching Organic Chemistry to high school students. The idea is not to substitute the learning process of the class, but used the game as an extension to the existing learning methods. This means that the players should have some previous knowledge about the domain, because it doesn’t teach everything from the beginning. The game allows students to play with the concepts learnt in class. The game explores immersive Virtual Reality (VR) to add interactivity and immersion to the traditional methods, thus enabling the students understand to better the more difficult subjects and the more abstract concepts. The use of VR comes with the challenges to define proper interaction mechanisms with objects, which is extremely important in this project since the player will be (directly) manipulating atoms and molecules throughout the game. 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. This allows the implementation of interaction techniques that simulate the way we interact with objects in the real world.

2 Background

2.1 Domain

The domain present in the educational game that was developed focus on the basic knowledge that a high school student should acquire about Organic Chemistry. This knowledge consists on information about the organic molecules, their nomenclature, structural drawings, 3D structure, class and formula.
2.1.1. Discipline Topics

Since the target audience of this project are high school students it was necessary to know and understand what is taught in high school about Organic Chemistry. From this initial research the discipline topics focus on the bonding, structure and nomenclature of organic molecules, the fundamental groups, isomerism, organic bases and acids and 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 Virtual Reality and Games in Education

To understand how Virtual Reality can be used in education, it is necessary to understand how humans learn and improve their skills and capabilities. According to the constructivist theory by Piaget a person learns in real life by doing and improves his skills through practice on realistic tasks, meaning that there must be active learning to have improvement. Since humans learn by having experiences and by interacting with their environment, Virtual Reality becomes a clear choice to create educational games. When creating a VR game or tool, there are three aspects to consider: immersion, interactivity and multi-sensory feedback (Christou, 2010). Immersion means being enveloped or surrounded by the environment and the key benefit of this component is that ensures the feeling that one is really in the virtual world. Interactivity is the ability to control events in the virtual world using one’s body movements and having the world generate responses to them, and multi-sensory feedback 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, interact with it, generate solutions to problems presented and have responses from the world to those actions, all within a safe environment. There are studies that show that games have a positive impact in changes in perception, attention and spatial cognition. From the results of those studies, we can assume that games can have an impact in teaching, but creating a useful and fun educational game is not an easy task. There must be a balance between the educational purpose and the entertainment aspect for the game to improve learning and be engaging at the same time. Kiili (2005) proposes a model that links gameplay with experiential learning to facilitate flow experience. The base of this model are the challenges based on educational objectives provided in the game, and through a cycle of attempts of the player and feedback from the game, active experimentation is induced. From this, it is possible to see a parallel between this model and the constructivist theory.

2.3 Chemistry Games and applications

Most chemistry games, that exist to date, are more commonly card games or boardgames. There aren’t many video games that focus on Chemistry, there are more applications and tools. The main applications and games analysed, and the conclusions taken from them are:

- Groupica (game) - shows how to correlate elements to their group families;
- Elemental Periodica (game) - uses the information about an element for the players to find out what element it is and what is its name;
- MolyPoly- depicts how gestures can be used to interact with molecules with the help of a manipulation panel.

2.4 Objects manipulation in Virtual Reality

The interaction with objects within the virtual world is an important issue to tackle, it has a direct effect in the immersive feeling of the virtual environment, thus impacting the whole experience. In the game developed, the interaction with objects (atoms and molecules) is extremely important, and for that reason 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 the device.

Manipulation Techniques

There are several techniques that can be used for manipulating objects 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. Poupyrev and Ichikawa (1999) created a taxonomy which categorizes the different methods of virtual objects manipulation available at the time by analysing their characteristics. They defined two major metaphors for the techniques: exocentric and egocentric. In this project the focus will be on the techniques from the egocentric metaphor. Although there are many techniques used for manipulation of objects, there are two major categories: Virtual hands - 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; Virtual pointers - 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. Although this is an easier technique to use and more efficient, it can be subjected to inaccuracy due to hand jitter and the Heisenberg effect. For this project, the classical hand will be mostly used for the manipulation of objects, since they will all be close to the players, and he won’t have a large space to move around on.

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 (Richard, 1996). For this reason, the chosen replacement for haptic feedback was the combination of auditory and visual feedback.

3. Implementation

3.1 Concept

After researching and talking to a high school Chemistry teacher, the defined domain of the game includes the nomenclature, structural drawings and functional groups of organic molecules. The several parts of the domain are integrated in the different game modes available on the game. There were two main game modes defined which were the Normal and the Speed Run modes. Both use the

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domain in its 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 Gameplay. There were also four 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. Therefore these sub game modes are Build, Complete, Transform
and Multiple Choice. These types of challenges will be described in the section 3.1.2.

The game mechanics used in all 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 manipulate the created molecules.

3.1.1. Learning goals

One of the most relevant components to define are the learning goals which 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. The final learning goals 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
- Correlate molecular structure with the nomenclature
- Correlate conventional drawings of molecular structures with their 3D structure

3.1.2. Challenges

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 must 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; 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 must 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.

One of the things that was discussed with the teacher were how the exercises applied in this subject
solidify the concepts that the students learn. It was clear that the same type of exercise can be used
for different concepts. This means that the same challenge can be used for different learning
objectives, making them versatile.

3.1.3. Gameplay

Two main game modes were considered: Normal and Speed Run. 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, we
plan to have 50 levels. One level can have multiple challenges of the same type, or it can have
challenges of different types. The difficulty for this mode will increase as the number of learning
objectives tackled in the levels increases. The first 20 levels tackle a distinct learning objective at a
time, meaning that there are 4 levels per learning goal. The order of the learning objectives is
correlated to the order in which the students learn the different concepts in class. 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. 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, we plan to have 10 levels, each level with 5 challenges that the player must solve as fast as they can. All the levels tackle a distinct learning objective at a time, meaning that there are two levels per learning goal.

3.1.4. Scoring system

The scoring system of the game is based on two measures: number of attempts and number of moves. 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 sense to count the number of moves that the player performs until he reaches the desired molecule. For a Multiple Choice challenge 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.

3.2 Technical Implementation

The game was developed in three iterations: the first one focused on implementing the core mechanics, the second was needed to improve some of those initial mechanics, and finally, the third one had the main objective of implementing the gameplay components (levels and challenges) and some extra elements. One of the most important aspects implemented in this stage was the relationship between an atom and a molecule as objects in the game (figure 1). When two atoms are connected, a bond is created between them and a molecule is formed. Every molecule has a pivot, which is a gear that is used in the manipulations techniques to help the play interact with the molecules. The position of the pivot is the mean of all the atoms position with an offset on the x axis, which means the pivot appears always to the right of the molecule.

3.2.1. Core mechanics

The core mechanics were implemented in this stage, which are connecting atoms, translating and rotating molecules. For connecting atoms, there were two methods implemented, one that was based on distance and another that was based on touches. The method based on touches consisted on grabbing two atoms, one in each hand, and touch the atoms together. Each time the atoms touch each other, while the player is grabbing them, the type of bond increases, from single to triple bond. When it reaches the triple bond and the atoms touch each other again, it circles and goes back to a single bond. The technique based on distance starts the same way as the first method described, but after the atoms touch each other once, the player must define 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.

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.
Initially there were three different rotation methods implemented. For two of these methods the user needed to define the axis around which the molecule should rotate. The player could set the axis through two distinct hand gestures with his left hand, which vary according to the method being used, while the right hand grabs the gear of the molecule. One of those methods rotated the molecule automatically after the axis is defined and the gear is held, the other method had the same process has the previous method with the addition of having to rotate the right hand’s wrist to rotate the molecule. For the third method it wasn’t necessary to define an axis, the player needed to grab the gear with his right hand and grab one atom of the molecule with his left hand. He then should move the atom around the centre of the molecule, which would be represented by a small red sphere to provide a visual reference of where it is, making it easier to understand how the he had to 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.

From the results of the testing phase of the first iteration, the conclusion was that the preferred technique to connect atoms was the method that used touches and that for translating a molecule, both techniques were adequate for different scenarios. 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 and the focus on the second iteration was to improve these two techniques and test them again. After this second evaluation phase, the Rotation with Wrist Control was discarded, and the Rotation with Atoms was defined as the rotation method.

3.2.2. Gameplay

The gameplay was built around the core mechanics by structuring the game in levels, which include the different challenges, and the scoring system. We create the levels in a flexible way, allowing for easy changes without tempering with the code. This was made through text files that are parsed by the system and that can be easily changed. They have a specific structure that must respected to be loaded correctly. The challenges have their own specific name that must be used. Each challenge has its own structure because each has different components that must be provided. These structures must be respected for the level to be loaded with no problems. For some of the challenges it is necessary to present a molecule to the player, and for this reason, the game needs to have a database with the molecules that should be loaded in those challenges. The database is a collection of text files, each of them correspond to one molecule, which has information about the molecule such as: the position it should appear, the different atoms that it has and the bonds that exist between the atoms.

3.2.3. Scoring system

The scoring is based on the number of attempts and number of moves. The number of attempts is used with the Multiple Choice challenges, and grants maximum points for a correct answer in the first attempt and minimum points after the third attempt. The actions that are considered for the number of moves are: bonding two atoms, breaking a bond, picking a new atom, throwing a molecule or an atom into the trash and remove all molecules or all atoms from the scene. Each challenge defines a level of required moves, which is compared to the actual moves the player does to compute the score.

3.2.4. Audio and visual feedback

Audio and visual feedback were extremely important in this project. The first visual feedback added was a yellow outline to the atoms that it is displayed when the player grabs them. An extra outline in red was used to indicate when the player could not connect two atoms together. This red outline appears when a player touches two atoms together where at least one of them doesn’t have any more available bonds to make. The number of bonds that an atom can have are represented by small

3 A video demonstrating the game play and core mechanics can be watched in this link: https://www.youtube.com/watch?v=4wdTYYRPyVc
spheres around the atom, and each time the player makes a bond with that atom, the correspondent number of spheres 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.

4. Results

In the final test the users were asked to perform a tutorial to understand how the mechanics work and get an initial feel for the game. After a tutorial they were asked to solve a mini version of the Normal game mode and afterwards fill a questionnaire. This game mode was reduced to 4 levels, which are detailed in the figure 4 that shows the challenges they had and the learning goals they tackle. The challenges used in the test were shown to the Chemistry teacher to make sure that the content of the challenges was correct.

4.1 Users Sample

This test was performed by 25 users, 8 were high school students ranging from 16 to 18 years old, and the remaining 17 were college students ranging from 18 to 26 years old. 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. The college students 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.

4.2 Evaluation Goals

To understand if the game created fulfils 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 challenges 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.

4.3 Experimental method

On this test, the logging technique was 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. The questionnaire used was based on the Game Experience Questionnaire (GEQ) and the VR Sickness Questionnaire, 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.

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

Fig. 3. Levels the users were asked to perform with their challenges and the learning goals that they tackled.
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 about the scoring methods asked the users how fair the methods were and how
pressured they felt using them.

4.4 Logs

The number of moves and attempts that the users made to solve each challenge were compared to
the respective optimal number of moves and attempts. 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.

From the results of the analyses of the number of moves and number of attempts (figure 5), it is
possible to say that the high school students had an overall better performance than the college
students. This was expected because the high school students had learned Organic Chemistry very
recently while the college students 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 close to the actual difficulty displayed by the users. However, there were some
challenges were issues with the implementation caused big values that could have been much lower
had those problems not existed (they are further explained in the Conclusions). 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.

4.5 Questionnaire

From the analyses of the section of the questionnaire about Game Experience (figure 5), the
conclusions are that the users had a positive experience with the game. They felt immersed in it and
they felt skilful while playing it. This can indicate that the mechanics implemented helped 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. 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 college
students 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. Regarding the VR Sickness section, it assesses two
components which are nausea and oculo-motor. The results of both components show that the users
felt almost no discomfort after they finished the test.
4.6 Observations

All the high school students had fun while playing the game, some of them even said it at the end of the test. They also seemed focused on solving the challenges and were concentrating on finding out the answer without any help. Most of the college students had fun and enjoyed playing the game. Some 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 it more fun to learn about this subject compared to the traditional method.

4.7 Interview to a Chemistry teacher

To have the point of view of a chemistry teacher, an interview was made to a high school Chemistry teacher.

Q: What advantages and disadvantages the game has comparing to the traditional teaching methods on Organic Chemistry? A: It’s more appealing to solve the exercises through the game than through paper and pencil, however it requires more time to solve them.

Q: How would you use the game in a class about Organic Chemistry? A: 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 school has a room with all the required equipment, it makes the process easier.

Q: Does the game help to approach Organic Chemistry in a more entertaining way? A: Yes. Without a doubt, it is a good method to cement the knowledge in a fun way.

By analysing the answers given by the teacher, the game might be a good tool to be used in the classroom to help teach Organic Chemistry, since it might be able to bring fun and entertainment in learning the subject.
5. Conclusions

The result of this project is a functional, fun and interesting game that has potential to be a good educational game to be used in a classroom to teach Organic Chemistry. All the proposed mechanics were implemented, as well as the challenges, levels, overall environment and auditory and visual feedback. The results obtained were overall very good. All the users enjoyed playing the game and the need to solve the challenges correctly to gain the maximum number of points made them invested in learning the required concepts by themselves and understand more about the domain. It was possible to see the users that knew more about the domain were applying the knowledge that they already had, and when they made a mistake, they analysed why it was wrong and were able to understand how to correct it and solve it.

5.1 Future Work

There are several aspects that would enhance the game if they were implemented, but there are two that would be the most beneficial. The first one is implementing 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 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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References

Eylem Bayor. Developing and playing chemistry games to learn about elements, compounds and the periodic table: Elemental periodica, Compoudica and Groupica. J. Chemical Education, February 2014.