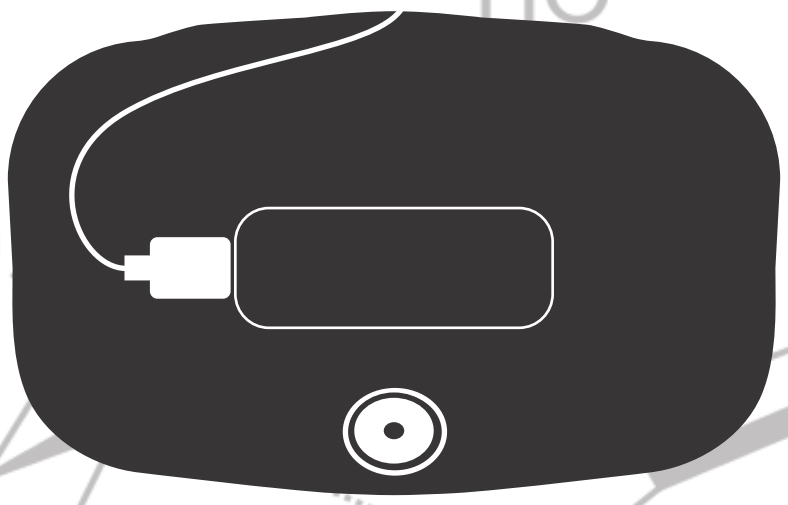
VR-CHEM

Developing a Virtual Reality Interface for Molecular Modelling



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Master of Arts Thesis

MA New Media: Game Design and Production

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Abstract

VR-CHEM is a prototype for a virtual reality molecular modelling program with a modern 3D user interface. In this thesis, the author discusses the research behind the development of the prototype, provides a detailed description of the program and its features, and reports on the user tests.

The research includes reviewing previous programs of a similar category that have appeared in studies in the literature. Some of these are related to chemistry and molecular modelling while others focus on 3D input techniques. Consequently, the prototype contributes by exploring the design of the user interface and how it can affect productivity in this category of programs. The prototype is subjected to a pilot user test to evaluate what further developments are required.

Based on this, the thesis proposes that 3D interfaces, while capable of several unique tasks, are yet to overcome some significant drawbacks such as limitations in accuracy and precision. It also suggests that virtual reality can aid in spatial understanding but virtual hands and controllers are far inferior to real hands for even basic tasks due to a lack of tactile feedback.

Keywords virtual reality, 3D user interface, molecular modelling

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1 Introduction

This thesis is about the development and testing of the prototype called VR-CHEM. The introductory chapter defines the prototype briefly, states the scope of the project including the goals and practical limitations, and finally outlines the structure of the thesis.

1.1 Prototype

VR-CHEM is a prototype for a molecular modelling computer program based on software that is commonly used by material scientists and pharmaceutical researchers. This version features two distinct interfaces. The first is a traditional computer interface with a mouse, keyboard and a monitor. The other interface is a novel, immersive, virtual reality environment with a head mounted display and a hand tracking input device. The program can employ either the Oculus Rift or HTC Vive virtual reality headset and utilises the Leap Motion controller for tracking hand movements and gestures. The prototype is capable of a selection of the most fundamental tasks that are required by professional modelling programs. Intended for user testing, the program has tools to record and report user actions.

1.2 Scope

This thesis is part of an Aalto Seed Funding project which is a collaboration between three schools of Aalto University: School of Chemical Engineering / Department of Chemistry and Materials Science; School of Science / Department of Computer Science; and the School of Arts, Design and Architecture / Department of Media. Professors at these schools have identified that current tools for molecular modelling in materials science are not optimal and that a combined effort could yield significant improvements. The first stage of this undertaking is the development of a working prototype that can demonstrate the capabilities of modern virtual reality technology and parallel 3D interaction. It also seeks to define the core feature-set of a molecular modelling program.

The goal of this thesis is to document the approach taken to design the prototype including the core features and user interface. With the limited time and resources, the prototype is not capable of replacing current tools for researchers but is useful for visualisation purposes. It is capable of importing molecules in certain common file types. Otherwise, it may be useful as teaching material for high school students who are learning about molecular structures.

1.3 Structure

In Chapter 2, we discuss the factors involved in such a program including an introduction to virtual reality and 3D interfaces. There is also a review of other projects that have attempted to use these new technologies. Chapter 3 has a detailed description of the prototype itself with the features and user interface elements. Chapter 4 covers the pilot user test, the results and some feedback from the test participants. Chapter 5 is the conclusion which tries to pull together the threads of the thesis and discuss some learnings. The appendix has additional data from the questionnaires of the user test.

2
Virtual Reality, 3D Interfaces and Examples

The great enthusiasm for immersive virtual reality (VR) in modern computer applications comes from the notion that virtual reality that mimics the real world would be more intuitive and effective for interaction than previous interfaces. This expresses itself in two main aspects: Firstly, virtual reality environments provide enhanced spatial and depth cues when compared with regular displays, leading to better visualisation and spatial cognition. Secondly, they afford for 3D interfaces or interaction devices with higher degrees of freedom than the standard keyboard and mouse. While studies (for example Doblack, 2011; Flores, 2012; Norrby, 2015) have shown that both these factors have had positive influences on user interactions, there are still questions about which particular use-cases justify the increased cost of the relatively sophisticated equipment.

One field that has exploited the advances in graphical and rendering technology is stereochemistry, which discusses the arrangement of molecular structures and substructures and how they change dynamically during chemical reactions. Several research groups have been using virtual and augmented reality to enhance their understanding of molecular structures. In particular, pharmaceutical scientists who aim to develop new drugs use such technology to immerse themselves

in the chemical reactions and observe protein structures, which are the target sites for said drugs. Also, materials science research uses state-of-the-art visualisation programs to study the properties of various metals and minerals.

2.1 Visualisation

Vision in humans is a complex phenomenon that involves the mechanisms in the eyes as well as the interpretation of the images formed in the eyes by the visual cortex of the brain. The brain can imagine space even with a simple 2D image but it becomes more accurate while perceiving depth and combining different perspectives. There are several ways of perceiving depth. In a simple example, an object appears smaller when it is further away. If an object seems to be getting smaller, given that it is not shrinking, one can assume it is moving further away and inversely they would seem increasingly large as they move closer. This is an easy effect to achieve in virtual environments and artists have employed this technique for centuries if not millennia. Another cue comes from the eye's accommodation or how the lenses in the eyes change their focal length – the muscles relax to focus on far away objects and contract to focus on nearby objects. While this aspect is often indicated in photography and films, the image is static once captured and does not respond to the viewers' eyes. Dynamic eye tracking and focus shifting in virtual environments is a more recent development. There is a new device called FOVE which is a virtual reality headset that is capable of eye tracking and artificial focus simulations (FOVE Website) but the projection plane/distance is still fixed so the eye lens is not changing focal length.

Stereoscopic vision refers to how the brain combines the images from both eyes and interprets it as one image with a sense of depth that is impossible with just one eye. It has greater impact for closer objects when you can literally see around the corner of one eye's view with the other. This is also where current technology is making greatest strides. In the last few decades, several techniques for delivering stereoscopic images have been developed and a few are discussed below.

Anaglyph 3D is an old method in which the images intended for each eye are colour-filtered differently (typically with red and cyan) and superimposed. When viewed through colour-coded anaglyph glasses, there is an illusion of depth. In a polarised 3D system, the different images are polarised orthogonal (linear)/opposite (circular) to each other and viewed though glasses where

the filter for each eye is also polarised differently. In active shutter 3D, the image source alternates between the two images while the glasses alternately obscure one of the two eyes. If the flickering is synchronised perfectly, the eyes are fooled into seeing the images simultaneously (Howard & Rogers, 1995).

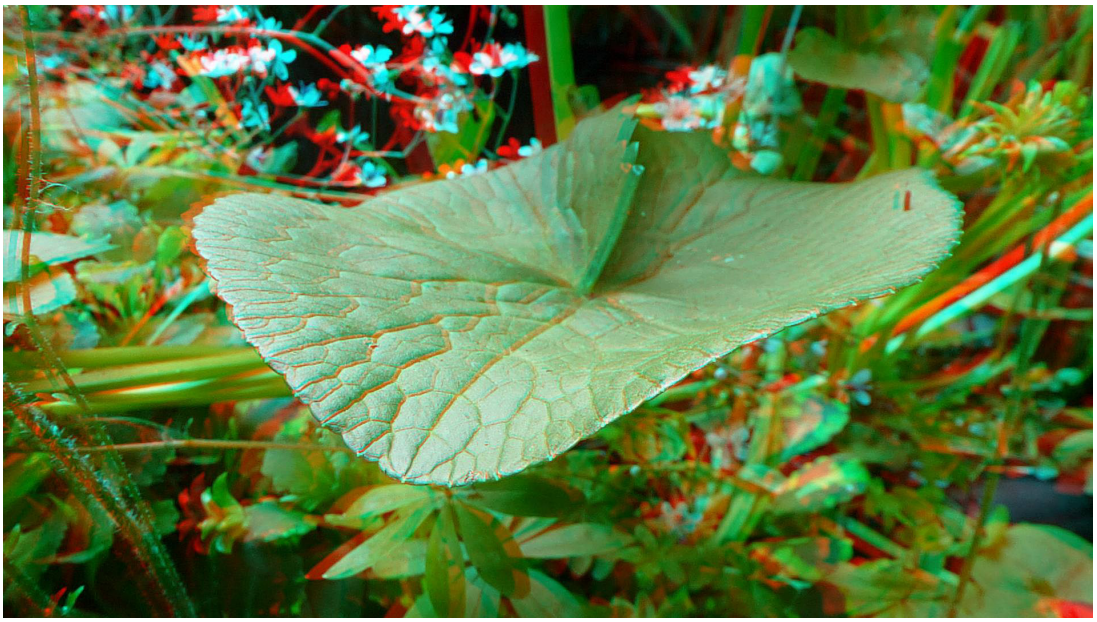

Figure 1. Red-cyan anaglyph 3D photograph

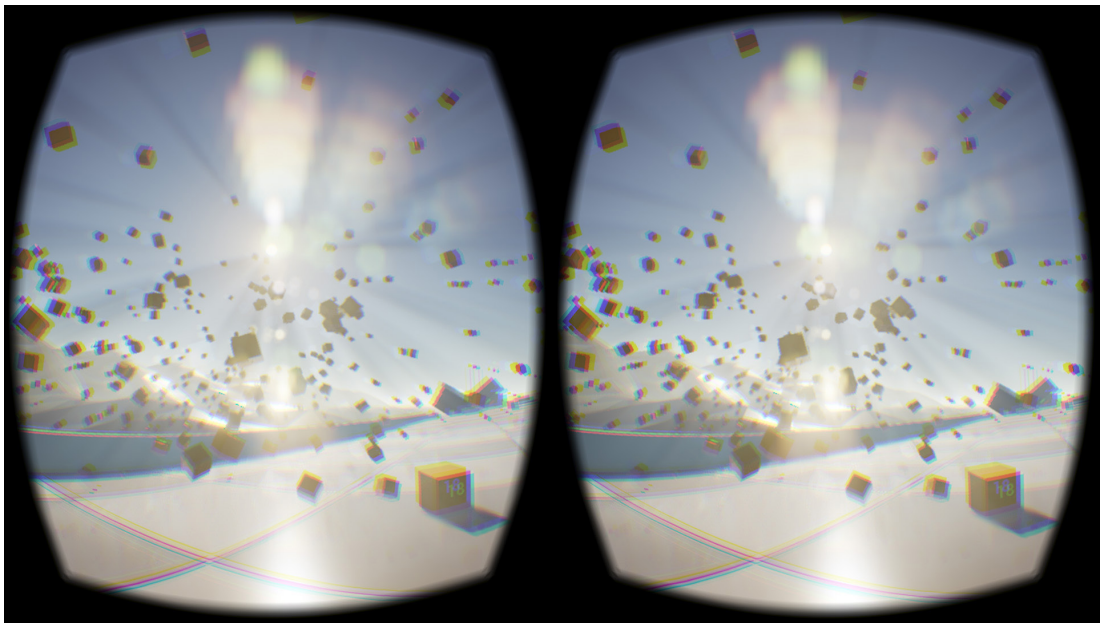

Figure 2. Different views for each eye in virtual reality headset

In current VR devices, there are two displays with different perspectives, one for each eye. They make use of a special lens that corrects the distortion of the image (the image is distorted and colour-aberrated intentionally beforehand) and increases the effective field of view.

Field of view (FOV) is one of the key features that enables immersion. Regular screens require a significant viewing distance to prevent eye-strain. As a result, even large screens occupy a relatively narrow field of view of the eye. Meanwhile, the lens in VR devices throws back the focal plane to a comfortable distance while being at a close proximity to the eye and occupying a much wider field of view. Higher end VR devices come close to the human eye's natural field of view and thus remove the sense of looking at a screen.

2.2 3D interfaces, degrees of freedom

The key to understanding the interest in 3D user interfaces is the concept of degrees of freedom. Degrees of freedom (DOF) refers to the number of independent parameters that are required to describe the state for a given object. In the context of spatial dimensions, the regular mouse provides 2 degrees of freedom, namely, the up-down axis and the left-right axis. The 2D plane on which the mouse moves is parallel to the ground but the reflected movement is rotated to a plane (the screen) perpendicular to the ground. This is due to the convenience of being able to rest the hand on the desktop while operating the mouse while looking straight ahead at the screen.

In 3D interfaces, a hand-held controller tracked in space can provide six degrees of freedom naturally. In addition to the third spatial dimension missing from the mouse there are the three rotational axes of the object, which are represented either in Euler angles or in a quaternion rotation. There are drawbacks in precision and comfort while handling these input devices. First, it can be tedious to hold up a controller instead of resting your hands on a desktop. In addition, with no resistant friction or vertical suspension, coming to a stable and stationary position for starting or ending a movement is more difficult, reducing accuracy and precision. Some of these problems are solved by using multi-DOF armatures and haptic pens. These can even simulate variable force feedback, which can have several uses. However, they are prohibitively expensive (Zhai, 1998).

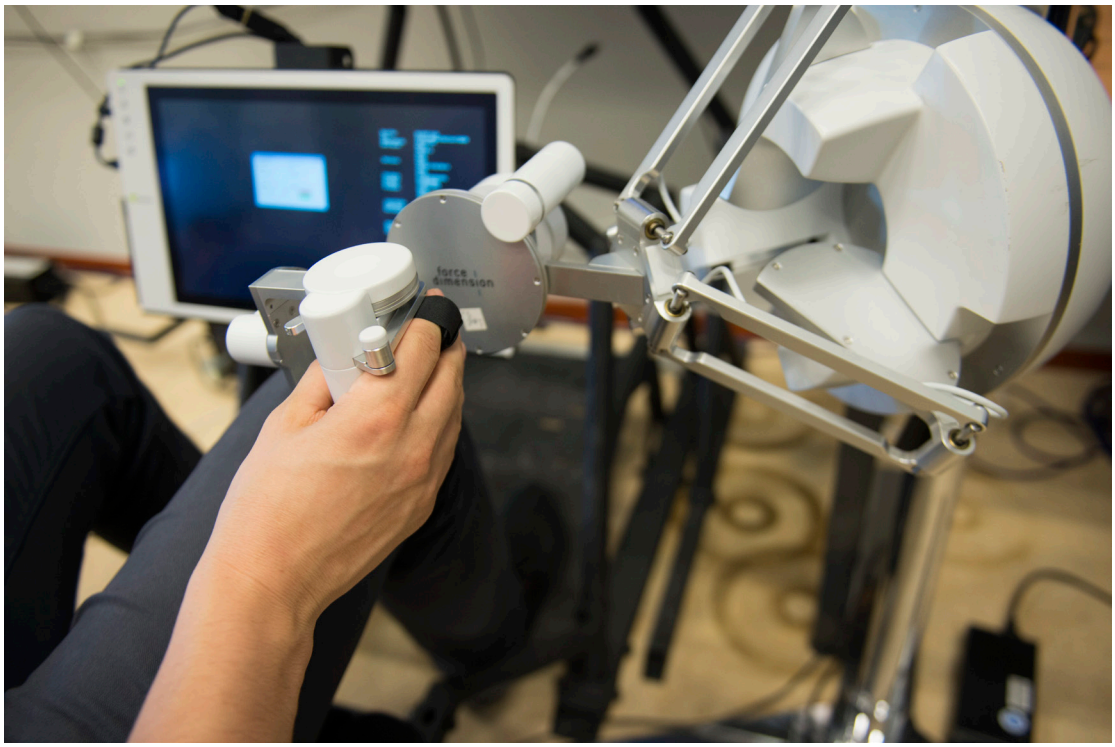

Figure 3. 3D input device for controlling robots

2.3 Current VR Devices

In virtual reality, the user wears a head-mounted device in which a stereoscopic display allows the user to see into a virtual world. Through head tracking (by an internal gyroscope, IR-LED tracking or with Valve's SteamVR Lighthouse system), the user's movements can be duplicated onto the virtual cameras, which in turn updates the rendered view and gives a sense of natural, realistic movement. In this way, they can traverse and visualise a 3D graphical environment. With the use of hand-held controllers that are also being tracked in space, there is potential for the user to manipulate objects in the virtual world.

The leading virtual reality devices are the Oculus Rift, HTC Vive, PlayStation VR, Samsung Gear VR and the Google Cardboard. The high-end devices have sold hundreds of thousands of sets already and the low-end ones have sold millions of sets worldwide. The industry is expected to grow to several billion dollars in the next few years. HTC claims it has sold well over the widely reported 140,000 sets as of late 2016 (Lang, 2016). Studies from SuperData Research (2016) indicate that Google Cardboard has sold tens of millions of sets and can turn smartphones with inbuilt gyroscopes into a display for a basic VR experience.

2.4 Augmented and Mixed Reality

Augmented reality does not remove the user completely from the real world as virtual reality does. It overlays images and data onto the view of the real world, thereby enhancing the user's experience of what he/she sees. In many ways, this can be more challenging because of how the computer has to interpret what the user sees.

When Google Glass was released in 2013, it was covered widely by the media but was plagued with legal issues. Augmented reality has existed for a long time but the Glass brought it into the mainstream. It was an unsuccessful product that was discontinued in 2015 (Lardinois, 2015) but it gave hope for a ubiquitous AR experience in the near future. This has been a mainstay of science fiction for generations.

More recently, Pokémon GO became a worldwide sensation. It was essentially an augmented reality experience where virtual Pokémon characters were scattered around and discoverable in the real world through a GPS tracked mobile device.

Figure 4. Mixed reality with the Hololens

When aspects of virtual and augmented reality are combined, they are referred to as mixed reality. Microsoft's HoloLens is a mixed reality device which is capable of interpreting the real

world as well as projecting virtual objects for the user to see. It has a few advantages over a purely VR device and some technical limitations.

The greatest advantage of the Hololens is that it doesn't impede the user's ability to perform regular tasks as immersive VR would. This allows the device to be worn for longer periods of time continuously. It allows for access to other interfaces simultaneously so that the user can read his/her screen, refer to handwritten notes, or even use a keyboard and mouse to interact with the virtual world more easily.

On the other hand, it does not provide nearly as much immersion with a significantly narrower field of view. The distances at which virtual objects are projected is static at around two meters distance from the user (Hachman, 2016). This is more obvious to users because looking at real objects will pull the virtual objects out of focus.

2.5 Limitations of VR

In the past, researchers (Robertson, Card, & Mackinlay, 1993) have regarded non-immersive VR (3D environments viewed through a regular screen) to be sufficiently immersive while being significantly more productive because the user can use the mouse and keyboard. The claim is still valid that these traditional input devices are dominant in most fields and merely the familiarity with them can compensate for any proposed benefits of immersion. There is a genuine concern that the novelty of head mounted displays with improved visual resolution can distract researchers from developing actually fruitful interfaces. There are also ways to produce stereoscopic vision without cumbersome head mounted displays (HMDs). The same effect can be produced with a 3D television and head tracking. Although they may not have as wide a field of view, these alternate methods can be used for longer periods before becoming a hindrance.

Another limitation of VR is how they are used in classroom environments (or for groups in general). Only one student can experience the full immersive environment at any given time. Perhaps in the future, all students can peer into the virtual world together but for now, it is a lonely experience. Additionally, the VR interfaces must be significantly accessible for non-technical instructors in order to implement them in education with any degree of confidence (Huang, Rauch & Liaw, 2010).

A lot more conclusive evidence through user testing and performance studies must be produced before a solid pedagogical foundation can be laid for VR (Huang et al., 2010).

Many experts agree that VR will be the next big thing in computing and can fundamentally change the way people relate to learning and working. The technology is still limited in several ways. The means by which users can interact with virtual objects is still 'primitive'. However, as several multi-billion dollar companies such as Facebook, Samsung, and HTC have invested in growing the VR market, one can expect steady growth of visual quality and creative leaps in user interfaces.

2.6 Examples of Previous Work

It is critically important to study previous attempts at creating a suitable interface that deals with manipulating objects in 3D space. This section will summarise some examples that are obviously not exhaustive of the possibilities but cover an important subset of them. Some of these are within the different fields of chemistry and they show the potential capabilities that VR-CHEM seeks to recreate. They also expose some gaps that this thesis addresses more widely. There are also examples from the fields of 3D models, animation, and data visualisation. Experts have weighed in on the applicability of VR in their fields respectively.

2.6.1 Examples in Chemistry

In some ways, the rendering capability of high-end computers puts virtual reality on the "brink of actual reality" (Morrison, 2016). There is a growing anticipation of using it for several educational and industry purposes. It can be a safe alternative space for experimenting with dangerous materials and environments. VR has the potential to revolutionise the approaches to chemistry in education. It moves molecular visualisation from 2D on-screen to 3D in virtual space. John E. Stone (Urbana-Champaign as cited in Morrison, 2016) predicts a massive surge in the use of VR devices in several fields and foresees their practical application in understanding and working with molecular structures. He has developed one such application called Visual Molecular Dynamics (VMD) for "large biomolecular systems" (Theoretical and Computational Biophysics Group, Urbana-Champaign [TCBG-UIUC] website).

Bell & Fogler (1995) have documented the effectiveness of virtual reality in education with a focus on chemical engineering. They suggest that it serves students who may not benefit as much from traditional learning materials. They do note an important limitation that persists over 20 years to the writing of this thesis: text-rendering inside the immersive VR environment faces severe difficulties.

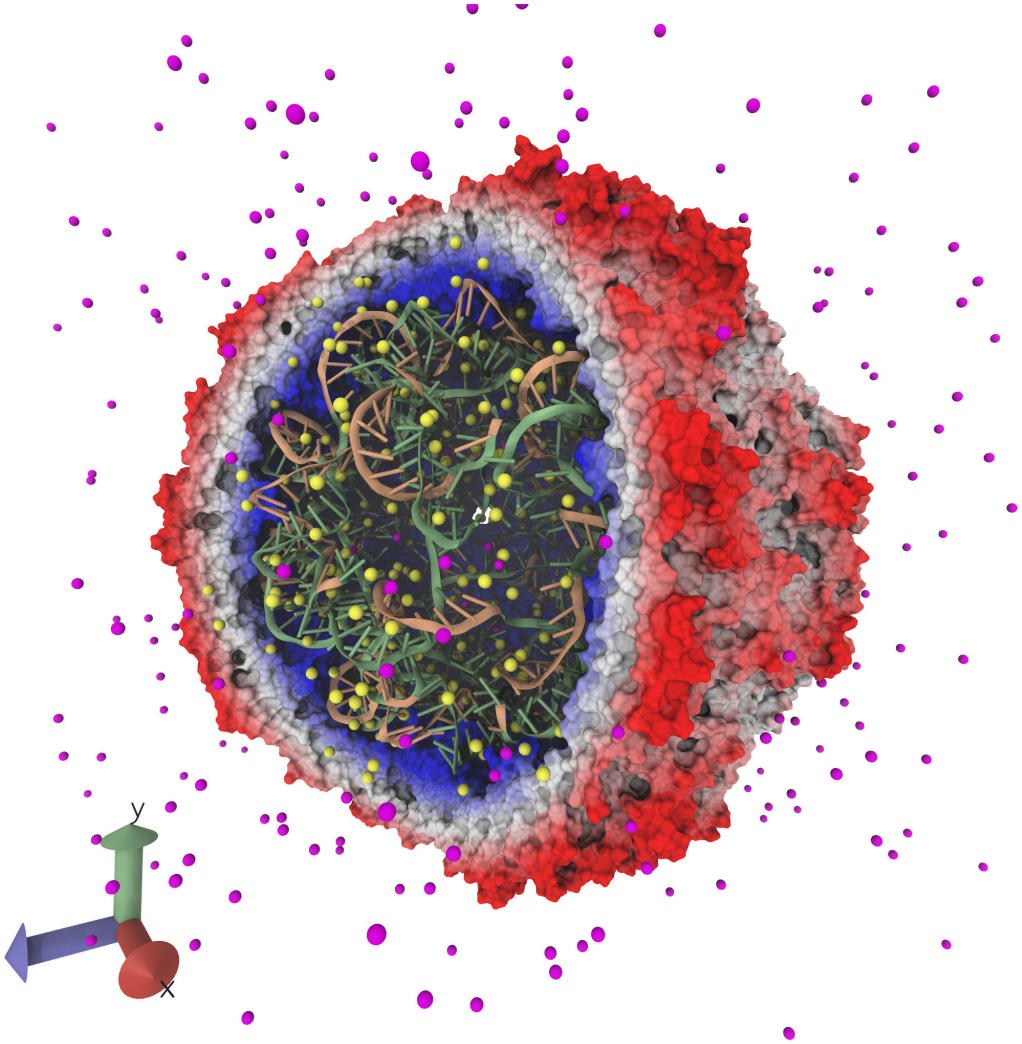

Figure 5. Satellite tobacco mosaic virus (STMV) rendering produced by VMD and Tachyon

The need to visualise a 3D molecular structure is at the foundation of the work that drug designers and many other scientists engage in – examples like ligand-protein docking, crystallography data, chemical shifts in NMR. In the past, various stereoscopic-3D effect techniques have been used but none have the immersive quality of virtual reality. Rester (2008) recounts that advances in visualisation technology have increased efficiency of identifying viable pharmaceutical drugs in

conjunction with various other optimisation methods.

These suggestions, insights and predictions have been prominent in studies for several years and are finally coming to fruition.

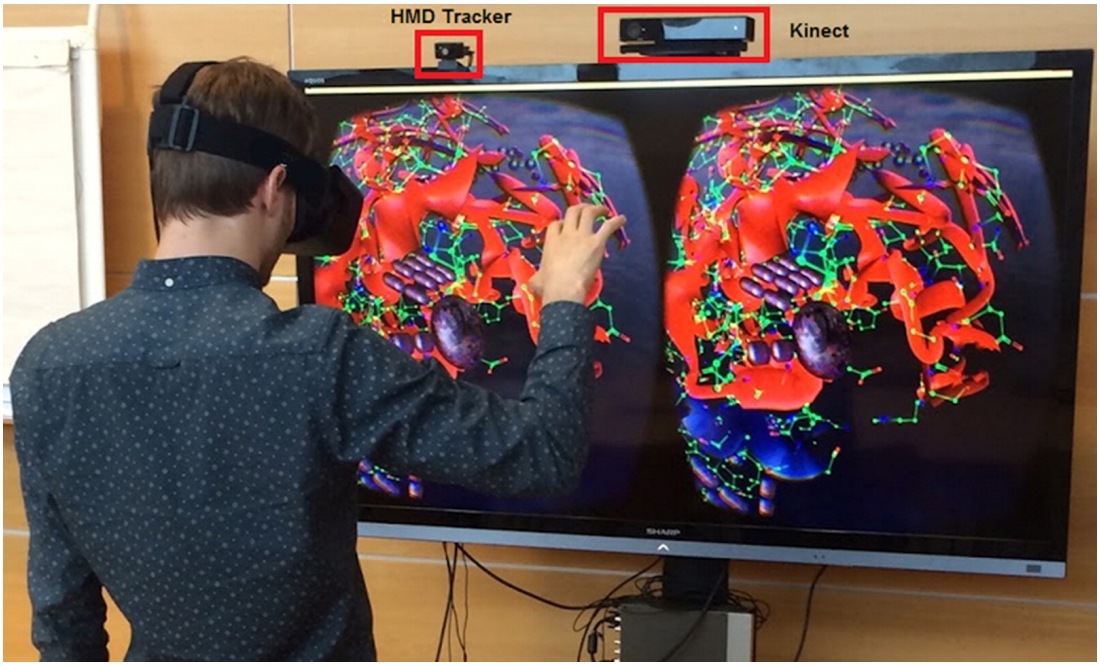

Figure 6. Molecular Rift

Molecular Rift

An example where VR is already being used in molecular model visualisation is Molecular Rift which uses the Oculus Rift and Microsoft Kinect v2. The team behind it has written extensively about their observations from several user tests with the application. Molecular Rift was used both to showcase how this technology could be used in industry purposes as well as in educational scenarios. In the application itself, the molecular data is manipulated using the Open Babel toolkit functions. There are several viewing options (lines, ball and stick, CPK colours). For protein secondary structures, ribbons can also be visualised. For alpha-helixes, StarManta's TubeRenderer was used for smoother curves. Intermolecular hydrogen bonds were depicted with a particle system rather than an actual solid object like other bonds. Certain pharmacophore elements were also highlighted. These are the features of a molecular structure that indicate the types of biological or pharmacological interactions that occur (Norrby, Grebner, Eriksson & Boström, 2015).

In 2015, the Kinect for Windows v2 had inbuilt hand gesture recognition for three of the four

symbols they used in their application: the open hand, closed hand and lasso gesture. The thumbs-up gesture is something additional. All the gestures used in Molecular Rift are a combination of these for both hands.

Using different focus groups for user testing, they were able to evaluate different features of the application and their usability. One group with more knowledge about chemical research who had experience with similar tools was used to understand how well the required features were implemented and whether they would serve their purpose in a lab. Other larger groups had more general participants and this data was used to improve the user interface and experience. They realised that they had to prevent unintended gestures from being recognised and fine tune the controls to make them easier to execute.

The results showed that the VR experience was more immersive due to the wider field of view and head tracking which simulates realistic movement in virtual space. However, the tool still lacks many of the core features that are present in more mainstream industry tools. For example, building molecules or performing force field calculations for energy minimisation.
There is also speculation that gamification of chemistry could encourage more students to pursue it academically (Norrby et al.,2015).

MoleculE VR

MoleculE VR is a smartphone application with VR support for viewing complex biomolecular reactions in cells. However, it is a more casual implementation and seems more effective for encouraging students' interest in biology and chemistry than for actual work. It is also an affordable entry for VR in cases where more equipment is not viable.

Autodesk Molecule Viewer

Autodesk has a VR-capable molecule viewer simply called Molecule Viewer. It can be used online as a web application with VR support and also imported to a smartphone application where it can be viewed through a VR device like Gear VR. The application can import Protein Data Bank (PBD) files and create snapshots or capture animation sequences. It has a very clean interface and a small set of easy to understand options for visualisation. It lacks more advanced manipulation and

molecule building tools.

This is a recurring theme: solutions for molecule or protein visualisation are spreading rapidly. There are only a few groups that have worked with input devices to interact with these molecules in a more rigourous way.

Materials Science at UC Merced

A materials science research group at UC Merced has developed a VR-like program for studying the structre of carbon nanotubes and other materials. They find that "[s]patial intelligence plays an important role in the success of nanoscience students specific to their visual ability to perceive structures in three dimensions" (Flores, Matlock, & Dávila, 2012).

In this project, the researchers have used a 3D TV, infrared head tracking and a Wii-mote controller to produce an immersive experience. The program was capable of some building and manipulation but more impressively had realistic physics simulations for inter-atomic forces. In a study, the participants were introduced to carbon nanotubes (CNTs) with different learning material, including virtual models. Cognitive scientists were involved in testing which methods were most effective in engaging the learners and which contributed to accuracy, interactivity, and understanding. With physical models, there was increased motivation and interactivity, but limitations in manipulating the structure. In a visual exercise, participants showed "improved visual ability" while observing the CNTs in the VR setup. (Doblack, Flores, Matlock, & Dávila, 2011).

The quoted cost of the setup was around $7000. This was published in 2011 before the tremendous growth of affordable virtual reality devices. The software used included Virtual Reality User Interface (VRUI) and Nanotech Construction Kit (NCK).

The limitations of this setup apart from the cost is the limited field of view and some reported dizziness. A large screen with stereoscopic 3D must still be viewed through 3D glasses and the resulting image is still rather small. In modern headsets, the field of view is significantly larger. Both the Oculus Rift and the HTC Vive have a 110 degree FOV (and more expensive prototypes like StarVR claim even wider angles) while even a large TV screen is optimally viewed at between 32 and 40 degrees (Optimum HDTV viewing distance as cited in Wikipedia, 2017). That is why the NCK is often used with a CAVE (KeckCAVES) environment where the entire room becomes the

screen and this delivers a level of immersion comparable with VR devices.

Quantum mechanical rational compound design (QM-RCD)

In a more recent project, the QM-RCD lab in University of Basel has developed a virtual reality visualisation tool for "immersion in electron density of drug-target complex" with the HTC Vive. Using the hand-held controllers, they are able to move and rotate the molecule, move the light, and utilise a virtual intersecting plane to observe the electron density in any cross section. An interesting observation from their studies was how manipulating the light's brightness as well as its direction was found to be quite useful for discerning a better sense of the 3-dimensional nature of the molecule (QM-RCD).

Haptic and Interactive Quantum Chemistry

The Laboratory of Physical Chemistry at ETH Zurich have developed a program for experiencing haptic feedback in chemical reactions. Although not an example of virtual reality, this is an example of advanced 3D input devices and real time quantum physics simulation. It makes use of a 3D pen with multiple degrees of freedom and haptic feedback to simulate quantum forces on atoms within molecules. The user can explore the potential energy field and "potential reaction paths" while molecules are undergoing chemical reactions. The forces are calculated from quantum mechanical first principles (in real time) rather than a classical force field so that no extra "parameterization for specific chemical situations" is required (Haag, Marti & Reiher, 2011; Haag, Vaucher, Bosson, Redon & Reiher, 2014; Haag & Reiher, 2014).

2.6.2 Animation, 3D modelling examples

Another field in which 3D interfaces have been explored to some degree are human animation tools. The joints and limbs of a human character model are transformed and rotated to create poses. This can be useful for games and animation sequences.

In one study (Kytö, Dhinakaran, Martikainen & Hämäläinen, 2017), an application was created for adjusting poses on a 3D human character with a 3D interface. The input was given through a combination of a regular mouse for selecting target body parts and non-tactile hand

gestures interpreted by a Leap Motion device for moving and rotating those body parts. But the mouse could still be used for the same actions as in classical 3D software for animation. It was discovered that while the mouse was better suited for fine tuning, hand gestures with six degrees of freedom was faster for achieving an approximate pose by controlling body joints and inverse kinematic (IK) end-effectors.

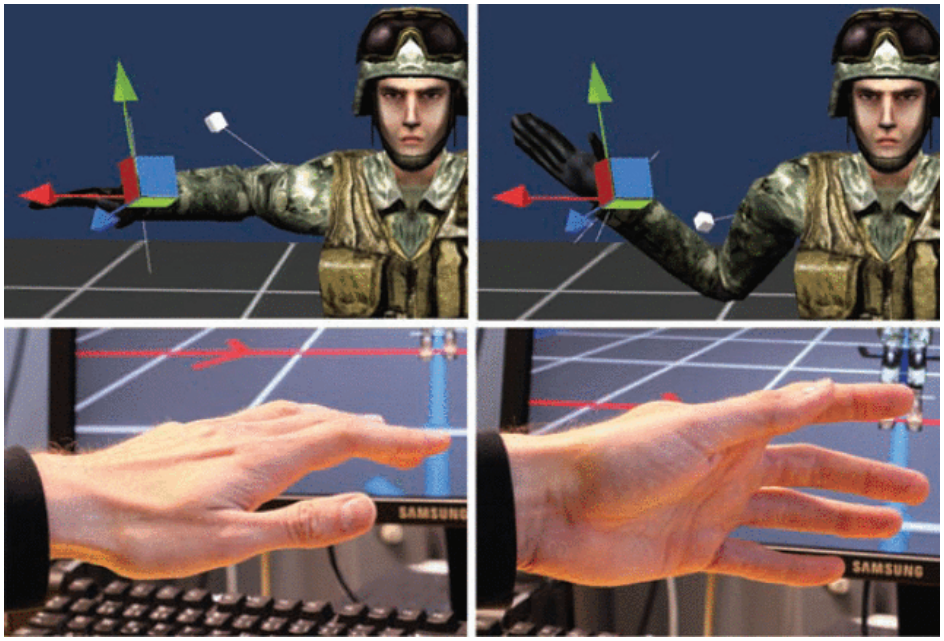

Figure 7. Rotating joints using hand tracking

Another approach to controlling human character models is through a virtual puppet-string-like system. Rather than selecting the joints individually, each hand and certain finger movements manipulate different parts of the virtual 'puppet'. The application developed for this study (Oshita, Senju & Morishige, 2013) showcased the potential of this system with the Leap Motion controller. Rather than just set a pose for the character as in the study discussed above (Kytö et al., 2017), they could be animated in real time. However, the range of possible animations was quite restricted. It was discovered through user tests that readings for finger bending angles were not stable because the Leap Motion device could not always track them accurately. Additionally, controlling real puppets requires practice and the interface devised here was equally demanding.

In a similar study (Luo, Lin, Chen, Yeo & Li, 2011), a virtual glove puppet was simulated which could be controlled by the user's hand while wearing a SmartGlove.

It is interesting to note that some of the problems that Leap Motion programs face can be tackled with glove controllers. The same gestures would be recognised more dependably because the fingers would not be eclipsed from the sensor by the other fingers. They are also more convenient than hand-held controllers as they weigh less and can be worn while working with real objects as well as virtual ones.

2.6.3 Other Examples

Other than education in chemistry, augmented reality has been tested in teaching geometry. One study (Kaufmann & Schmalsteig, 2003) experimented with this new format in a test with school students. The assumption was that interacting with 3D objects in a 3D virtual environment can increase understanding and intuitiveness. This did seem to be effective for certain spatial reasoning tasks.

There are great expectations for document and data navigation in 3D and VR. In today's information saturated world, it becomes increasingly relevant to handle and process data in faster ways. There are no cross-platform, hyper-linked meta-data structures that can help the researcher browse information based on concept spaces. The internet is superior to a library but it has not reached its potential given the available resources and technology. A "multidimensional document proximity space" (Ihlenfeldt, 1997) would be revolutionary in this broad discourse.

Needless to say, there are fantastic possibilities for immersive narratives and games.

2.7 Taking it Forward

The examples discussed have revealed some possible issues in moving forward. It is crucial to lay them out and dissect them in order to proceed with developing a new program.

One of the pressing limitations is cost-effectiveness. Perhaps some well-funded research labs can afford advanced 3D haptic pens with 6 degrees of freedom. From an education perspective, it might be pragmatic to consider what a classroom can reasonably afford. If virtual reality has a role in the future, which seems likely, it might be feasible for schools to invest in a setup, especially as they can cost below $1000 and will get increasingly inexpensive with each year. Educational institutions will probably have VR rooms in the next few years just like any other specialised

equipment or screening rooms covered by their A/V budgets.

Another matter is that virtual reality interfaces are evidently not suitable for long periods of use. The head mounted displays are cumbersome and holding up 3D input devices is tiresome. Therefore, the first requirement would be to make an application that can be used even without those devices. Indeed, the ideal scenario would be a seamless integration between regular usage in a standard setup and a VR setup. Then, the user can spend dedicated time in the VR environment to get an understanding and play with elements but can also sit down at a desk and continue with a less intense session.

An alternate solution would be an augmented reality interface like the Microsoft HoloLens that would allow the user to use multiple input devices freely. There would be a higher degree of calibration to be done beforehand but the result would be a more seamless workflow. The user would have access to the real and virtual world simultaneously.

It is clear from the examples using Leap Motion and Kinect that finger gestures are extremely limited and unstable for a productive, professional work tool. However, it presents itself as a more elegant solution and may become an intermediate input device before smart gloves or VR glove controllers become more accessible.

After studying the common features of traditional molecular modelling programs like Avogadro, jMol and ChemDoodle, a list of required functions for the new prototype was formulated.

- Creating molecules by adding or subtracting atoms and bonds
- Arranging, moving and rotating sub-structures of molecules
- Stretching and shrinking bond lengths
- Showing ball-and-stick figures, CPK colouring, secondary structures
- Measuring distances, angles, torsion of and between bonds
- Carbon atoms automatically adding hydrogens (saturation), ability to replace a hydrogen with something else.
- Offering a short list of elements to choose from, with a button to open a whole periodic table

Many of these functions are present in the prototype. These are discussed in detail in the following chapter.

3
Prototype

VR-CHEM is a prototype for a molecular modelling program that integrates different user interfaces. It was proposed as part of a seed-funded collaborative research project and it continues to be iterated upon beyond the time frame of this thesis. Its two main developers are master's degree students from the School of Arts, Design and Architecture and the School of Chemical Engineering in Aalto University with additional input from the School of Science, Department of Computer Science. I worked primarily on designing the user interface and interactions while Otso Pietikäinen was responsible for the scientific accuracy of the atomic interactions.

The prototype was built with the Unity 3D game engine. It makes use of input from a Leap Motion controller, and is compatible with both the Oculus Rift and HTC Vive virtual reality headsets. The Leap device is mounted on the headset to track hand movements and gestures while the user is immersed in the virtual environment. VR-CHEM can also be used with the standard mouse and keyboard inputs. Typically, a full-fledged molecular modelling program allows the user to create complicated molecular structures, manipulate them and ascertain details about their geometry. The user is able to observe the relationship between different sub-structures or multiple

molecules. The prototype discussed here is able to perform the most basic of the tasks mentioned and demonstrate the advantages, and perhaps some disadvantages, of a virtual reality version of such programs.

3.1 Feature Set, Choosing an input device

Designing the user interface for VR-CHEM was both exciting and frustrating at the same time. The process demonstrated the great potential of virtual reality and 3D user interfaces while simultaneously uncovering the limitations, inconveniences and challenges that developers and end users may face.

The first stage of development involved defining the scope of the prototype: Which features were most instrumental in forming a proof of concept for 3D interaction and to what depth the user interface needed to support such features. It was clear from the beginning that this would be more than simple a visualisation software. Such software is already quite common in chemical engineering and pharmaceutical research. Apart from being able to observe a molecule in stereoscopic 3D, it was essential that the user be able to create, adjust, and fine-tune details such as the bond length, bond angles, and atom saturation.

The first major decision in designing the 3D user interface was selecting a suitable input device. Keeping in mind the availability of such devices in the market in case the program is to be used in education and research, there were only two viable options. One was the Leap Motion controller, which is able to detect the user's hand movements and gestures, effectively making the hands themselves input devices. The other was the hand-held controllers that come packaged with the VR headset: the HTC Vive's controllers or the Oculus Rift's Touch controllers. While the controllers are better tracked in 3D space and have more accurate button presses (indicating that an action is being performed) they are heavier, more cumbersome and do not offer flexibility of gestures. The appeal of a simple interface with just hand gestures seemed the better option at the time. Therefore the Leap controller mounted on a VR headset presented itself as the preferred input method. However, in retrospect, I would reconsider this choice strongly. The low precision of 3D interfaces in general is further let down by inaccurate tracking which was a problem we faced repeatedly in the course of development. Also, while the hand is theoretically capable of a

multitude of intricate gestures that far surpasses any set of buttons and triggers, it is less justifiable to rely on hands when only a few common gestures are easily registered by the device.

In the initial versions, the interface consisted of several discrete modes each for a small set of related actions. For example, to create new atoms, there was a creation mode, to measure the distances between them, there was a measurement mode. This is not considered good interface design for modern applications because of mode errors: where the user performs the correct sequence of actions but in the wrong mode leading to undesired results. It is also not an elegant use of the gestural interface because switching modes involves interacting with a 'non-diegetic' interface like a virtual button that reads 'Create' or 'Measure'. While it is inevitable to have some state system which detects user input and performs appropriate actions, the fewer explicit modes, the better. Additionally, the state changes can be more intuitive when they are context sensitive. Thus, in later versions, the mode system was replaced. The state (of the aforementioned state system) would depend on which atoms and bonds were selected. For example, if a bond was selected, moving the adjacent atoms would stretch the bond. If two bonds were selected, one could be rotated towards or away from the other. The only downside to this is that the user is not presented with all the various possibilities at first sight but must uncover the state system layer by layer.

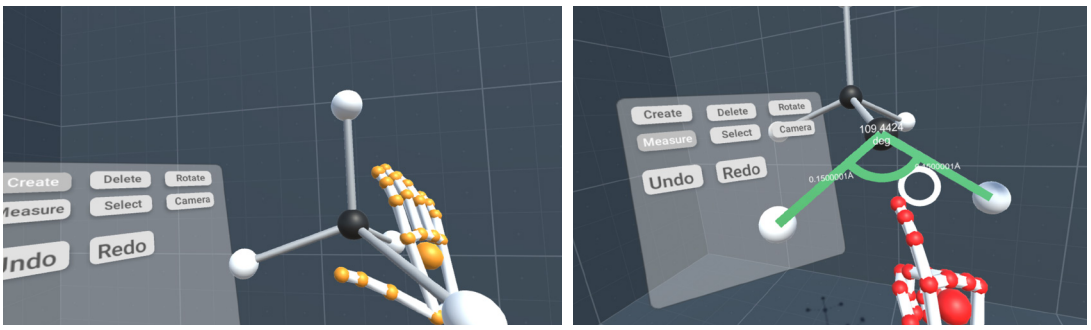

Figure 8, 9. Creation and measurement modes in early iteration of VR-CHEM

Having selected the Leap controller as the input method, the next step was identifying which gestures worked well and what actions they would correspond to in the program. The hand gestures that the Leap controller detected most effectively were pinching, grabbing and pointing. The pinching action involves holding the index finger and thumb together while other fingers were extended. The grab gesture involves bringing all the fingers together as though holding a small object

with them. The pointing gesture works with the index finger extended and all others closed into a fist. In a natural pose, the closest fingers to the eyes, and therefore closest the detector, are the index and thumb. The other fingers are somewhat obscured behind these. The Leap controller's sensors, while mounted on the headset, cannot clearly detect the obscured fingers' positions and this leads to glitches that disturb input consistency. The most common applications and games developed with Leap designate similar gestures for user actions. This suggests that they have experienced the same issues with other gestures and narrowed the possibilities down to the same few well recognised gestures.

Since the sensors were capable of distinguishing the left and right hands, there was the possibility of increasing the number of unique actions by performing the same gestures with the other hand. This lead to the dilemma of whether all actions should work with either hand or if they can have different meanings and effects. In some cases it would be convenient to have both hands perform the same actions. Firstly, it would mimic the symmetry of our hands in the real world. Similar actions with each hand would produce similar results. Secondly it would allow the user the have more reach to carry out a specific task in the virtual environment while stationary or seated. Lastly it would offer the user some rest for one hand while the other is being used. However, there is a counter argument. While our hands are symmetrical, people are often more skilled in certain tasks with different hands. They are indeed used asymmetrically in several demanding tasks. From using a computer where one hand is controlling the mouse, to playing musical instruments like the guitar with one hand on the fretboard while the other plucks the strings. Indeed, there were significant advantages to favour an asymmetrical interface and this was implemented in the prototype. However, there should have been an option to switch the handedness and this became more apparent in the user tests when a left handed participant struggled to execute the tasks.

3.2 Leap Gestures

The pinch gesture is designated to the 'create' action which has subtle variations that determine what is being created depending on where the action is performed. The pinch action has two sub-actions. The pinch from a neutral state and the release of the pinch. If both are performed on empty space, an atom is created at the pinch point where the fingers meet. If both are performed while

the pinch point is within another atom, that atom is replaced with a new atom. There is a panel with a list of elements that the user can choose from and this will determine which atom is created. Further, if the pinch is performed on an existing atom and the user moves the pinched hand to another existing atom to release the pinch, a bond is created between the starting and ending atom. If the pinch starts on an existing atom but is released on empty space, a new atom is created at the release point and this atom is bonded to the atom where the pinch began. Finally, pinching and releasing on an existing bond changes the bond multiplicity: it cycles through a single, double and triple bond.

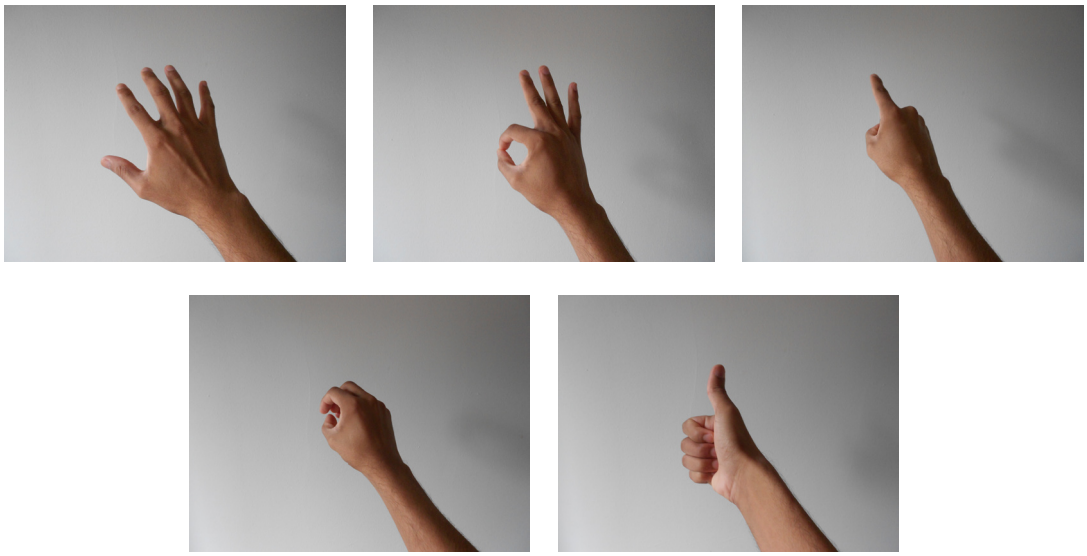

Figure 10, 11, 12, 13, 14. Hand gestures: neutral, pinch, point, grab, thumbs-up

Selection is performed by forming a pointing gesture and touching the selection target with the tip of the right index finger. There is a system by which selections can be changed or deselected: The first selection must be a bond. When this bond is selected, touching it again deselects it. If a bond which is not adjacent to the first bond is selected, the first selection will be replaced with the new one. If the bond is adjacent, the second bond is marked for movement. While the second bond is marked, selecting another bond which is adjacent to the first marks that other bond for movement instead. If a bond is marked for movement and the first bond is deselected, the marked bond will now take the place of the first bond as a selection. While a first bond is selected, if instead of selecting an adjacent bond, an adjacent atom is selected, that atom and its connected chain is marked for movement. And like the bonds, if the other adjacent atom is selected, that will

be marked for movement instead. Retouching the bond or atom marked for movement, unmarks it. Finally a thumbs down gesture with the right hand deselects everything. Although this seems convoluted, it is relatively simpler than the number of selections required for certain actions in current modelling software. For example a simple rotation may require the user to select four atoms in a row, three to establish the plane and angle around which the fourth rotates. In our prototype, by making a few justified assumptions about the axis of rotation being around a bond vector, the system becomes simpler by a few degrees.

The grab action is used to move atoms or groups of atoms. This too has many different meanings. It can be used for moving atoms individually, rotating atoms groups, and stretching bonds. It depends on what is currently selected. If nothing is selected, the grab action can be used to freely move an atom while keeping the rest of the molecule in its place. It maintains the connections to other atoms through bonds by stretching the bonds to the necessary lengths even if they are not the accurate distances. This can be used to fine-tune the position of atoms one by one. The remaining move actions require something to be selected.

If a bond is selected, it is highlighted in green and the two connected atoms are highlighted and outlined in yellow. The yellow outline generally indicates which objects can be acted upon or moved. Grabbing and moving one of these two atoms stretches the selected bond while maintaining the bond direction/vector and not affecting the configuration of the remaining structures on either side. If after selecting a bond, an adjacent bond (that is, a bond connected to one the two highlighted atoms) is selected, the second bond is marked with yellow to be moved. It, along with the chain of atoms connected to it, will pivot around the atom which connects it to the first selected bond and it will pivot towards or away from that first bond. However, if the second bond is part of a ring, this manipulation is forbidden. Similarly, if after selecting the first bond, an adjacent atom is selected (that is, one of the two connected, highlighted atoms), that atom and any further chain of atoms and bonds will be marked in yellow and highlighted to be moved. This structure will rotate around the atom using the first bond as the axis of rotation. Again, if the atom is part of a ring, the manipulation is forbidden.

While all the other grab and move actions are performed with the right hand, there is one feature of movement with the left hand. The whole molecule or group of molecules can be rotated

around a center point. Using the left hand, the grab action can be used at any location and as the hand moves, the molecule will rotate accordingly around its visual center. This is a common feature of not only other molecular modelling software but also of several 3D design software. It allows the user to orient the molecule in a more comfortable way for interacting. It can help them see the molecule from different angles and also to bring closer whichever parts the user wants to act upon next.

There is also a thumbs up gesture that allows users to delete atoms and bonds with the tip of their thumb but it led to several accidental deletions and is being modified. There is an option to increase the area of effect of the deletion. It appears as a cube connected to the thumb and it deletes everything within it.

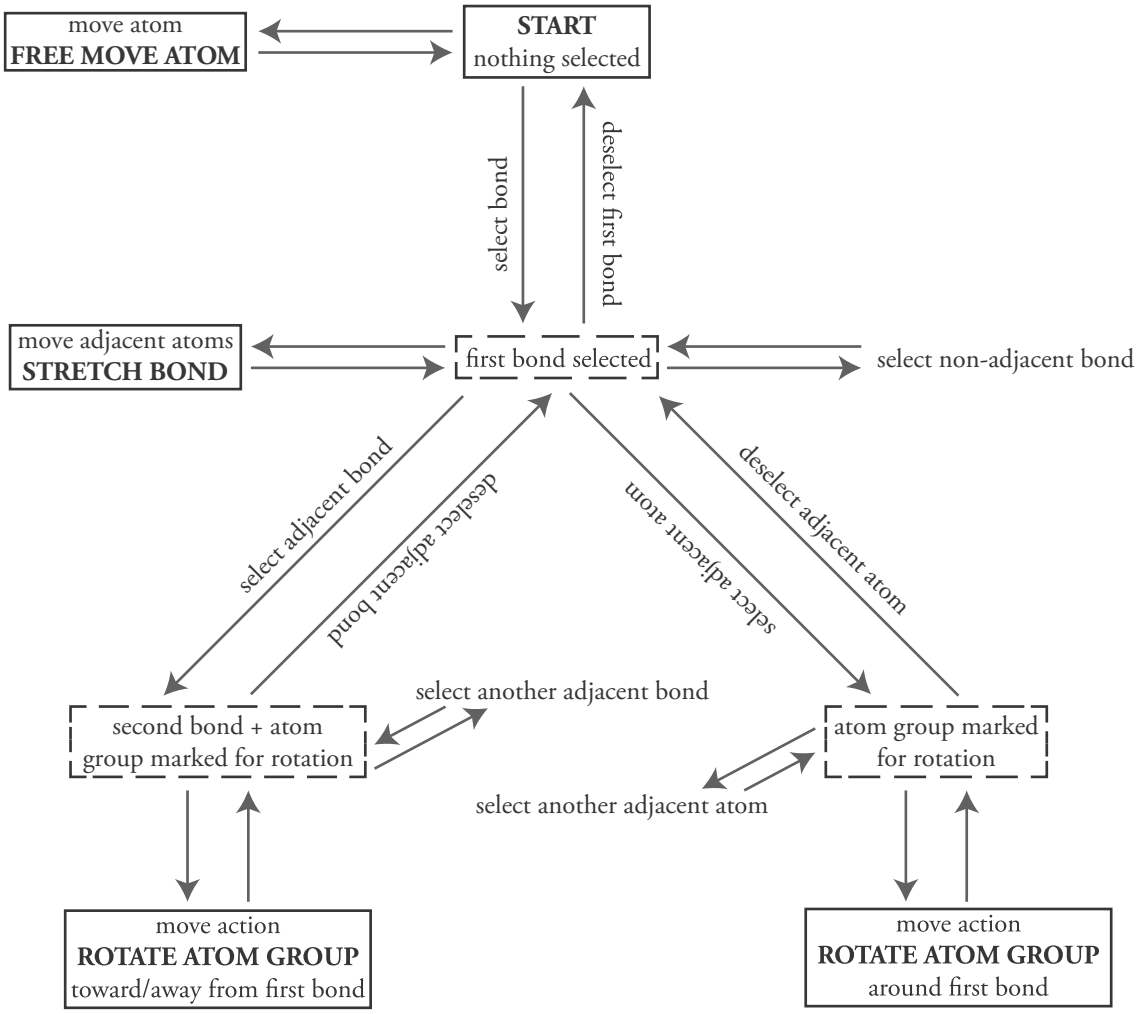

Chart 1. Selection states and actions

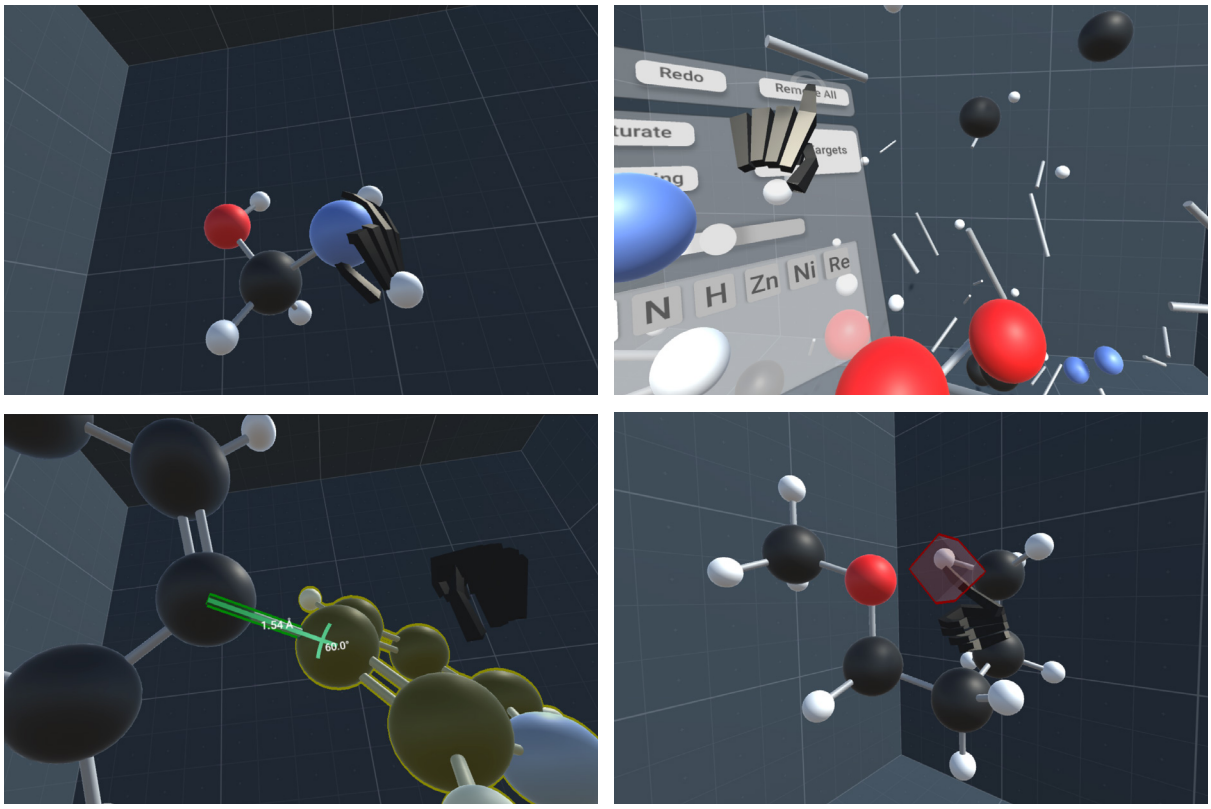

Figure 15, 16, 17, 18. Creation by replacing, Remove All button, Rotating atom group around bond, Deleting with thumbs-up gesture

3.3 Keyboard and Mouse Controls

The keyboard and mouse interface replaces the gestures with certain keyboard buttons and mouse clicks. The user can select bonds and atoms by clicking on them with the mouse pointer. To simulate the pinch action for creation or replacing, the user holds down the 'c' key while the mouse click-and-release works as the pinch-and-release does. To simulate the grabbing actions, the 'v' key is held down while the mouse is clicked and dragged. For deleting, the 'd' key is pressed and a red outline shows which target is to be deleted.

3.4 Panel

In both versions of the program, there is a panel for settings and inputs that are not performed directly on the molecule. In the VR version, the buttons on this panel can be pressed by either hand but it is placed slightly to the left of the player's view so it may be most convenient to use the left hand. That is also preferable due to the fact that the right hand may be used for most other actions. The traditional computer screen has the same options as buttons that can be interacted

with through the mouse pointer and some options were also given keyboard shortcuts.

The VR panel is significantly more inconvenient than keyboard shortcuts or mouse clicks which are tactile and reliable. There are buttons for undoing and redoing actions. There is also an option to clear the screen, in essence. In the actual program, when the 'remove all' option is selected, there is a short animation of the current molecule exploding and falling to the floor before disappearing but this serves no practical purpose.

There are also some basic options that change how the molecules are built. There is an option for whether the elements are automatically saturated with hydrogen atoms or not. There is an option for whether rotations are smooth or snap in increments of 15 degrees. In a future version, it would be convenient to be able to change the increment amount.

There is a slider to specify the size of the delete box. When the size is set to 0 or the smallest value, the delete action only deletes whatever is touched directly by the thumb or clicked on directly by the mouse. As the size increases, there is a 3D box for the VR version and a 2D box in the keyboard mouse version. Everything within them is deleted.

For the user to select what is being created, there is a list of common elements and a button that opens a full periodic table. The user can select any element from it and even add those elements to the main list if they are needed more often. For this prototype, the bond lengths and saturation details were only specified for a few of the most common elements used in organic chemistry. To expand the functionality, these details for other elements can be added to an external file which the program reads to adjust the bond lengths and angles.

4
User Testing

With a reasonably stable prototype showcasing the features discussed in the previous chapter, a simple pilot test was conducted in order to evaluate the usability of the 3D user interface by comparing it with the more traditional interface. The aim of this test was to qualify and quantify the ease of use and adaptation required for a small sample size of users when experiencing VR and 3D user interfaces. The results were expected to match what similar previous studies (Kytö et al., 2017; Norrby et al., 2015) have indicated: that for simple tasks requiring little precision, the 3D interface is effective, but as the task increases in complexity and demands more precision, there is a lack of consistency with 3D inputs. Here, the keyboard and mouse are vastly superior and extremely reliable even if they are limited in other ways.

Most participants of the test were master's degree students or doctoral candidates in some field of chemistry while others were game design and graphic design students who might have more experience with VR games and user interface design. There were 11 participants in the first set of tests that were conducted before the completion of this thesis. There were 9 male and 2 female participants ranging from 24 to 38 years of age.

We asked each participant to attempt three different tasks focusing on slightly different aspects of the program. They would each be performed with both a regular user interface using the mouse and keyboard and the 3D interface using the Leap Motion controller mounted on a HTC Vive VR headset.

4.1 Tasks

The first task was to create a molecule of "ethylene glycol", a simple diol, and to align the two hydroxyl groups if they are staggered. The test participant was shown a 3D model rendered from a fixed angle and asked to reproduce it. This task would require them to perform the create action, understand how to build a molecule by replacing hydrogen atoms, and identify which bonds form the axes around which atoms groups rotate.

In the second task, the participant was presented with a "3,3',3"-Benzene-1,3,5-triyltripyridine" molecule consisting of four rings: one ring in the center and three around it. The outer rings were coplanar with the central one and each had one nitrogen substitution. The task was to rotate the three outer rings around the connecting bond to be perpendicular with the inner ring such that all the nitrogen substitutions were on the same side of that plane, all above or all below. The molecule in this task was so large that it would be impossible to reach all the rings from one position. The prototype did not feature a scaling option. Instead, it demanded that the participant rotate the molecule and bring whichever section they wanted to act upon closer to them.

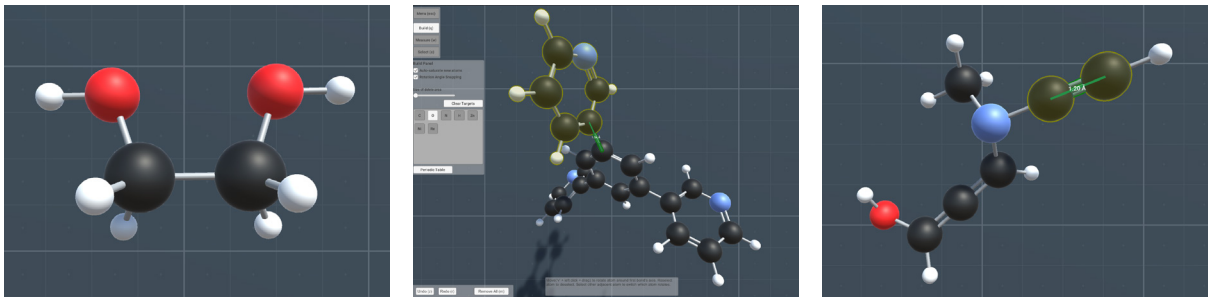

Figure 19, 20, 21. The molecules involved in the three tests

The third task required the participant to build a more complex molecule "3-(N-Methyl-N-ethynylamino)-1,2-propadien-1-ol" given its structural formula. Therefore, rather than being presented with a 3D model like the first task, they must translate the 2D graphical representation

that is typically used in the field of chemistry into a 3D structure within the program. It is natural that some additional guidance was provided for game design and graphic design students who might not know or remember how to read such a representation. The molecule required some bonds to be modified into double or triple bonds. But there was no rotation, movement or alignment required.

The prototype had an inbuilt method to record the time taken and number actions performed in each test scenario. It also recorded the number of 'undo' actions the user made. The results were noted for every test and compiled thereafter. Once reviewed, this data was largely in accord with the anticipated outcome with some exceptions.

The exercises were followed with a short questionnaire where participants gave their personal feedback about the program and certain broad features of the interface. First there were some questions where the participant would rate a statement from 1 to 10 where 1 expressed 'strong disagreement' and 10 expressed 'strong agreement'. After these statements were a few open-ended questions that required a few sentences of feedback and related comments. Additional information from the questionnaires is given in the Appendix.

Figure 22, 23, 24. Test participants

		Keyboard Mouse Interface			VR Interface		
Tester	Task	Actions	Undos	Time	Actions	Undos	Time
1	1	19	2	197	9	3	159
	2	7	0	87	14	0	114
	3	14	2	142	16	4	172
2	1	9	0	55	26	3	117
	2	7	0	52	14	0	200
	3	12	0	56	28	10	189
3	1	17	0	141			
	2	11	0	138		n/a	
	3	28	5	195			
4	1	8	0	111	28	0	143
	2	5	0	102	6	0	90
	3	21	0	139	21	0	156
5	1	15	0	112	21	0	115
	2	6	0	70	4	0	78
	3	19	0	65	32	0	77
6	1	8	0	70	15	2	125
	2	9	1	71	14	0	112
	3	27	0	159	15	0	87
7	1	10	1	76	14	0	59
	2	3	0	40	18	0	94
	3	12	0	48	82	0	216
8	1	10	0	206	32	13	410
	2	6	0	61	10	0	141
	3	11	0	114	28	0	328
9	1	8	0	197	17	2	94
	2	4	0	70	10	1	94
	3	12	0	48	15	3	107
10	1	14	3	226	7	0	71
	2	3	0	53	9	0	67
	3	15	3	131	24	6	111
11	1	14	0	198	11	0	110
	2	4	0	89	17	1	73
	3	13	0	173	13	1	86

Table 1. Results of user test

		Keyboard Mouse Interface			VR Interface		
Tester	Task	Actions	Undos	Time	Actions	Undos	Time
Average	1	12	0.5	144.5	18	2.3	140.3
	2	5.9	0.1	75.7	11.6	0.2	106.3
	3	16.7	0.9	115.5	27.4	2.4	152.9

Table 2. Averaged results

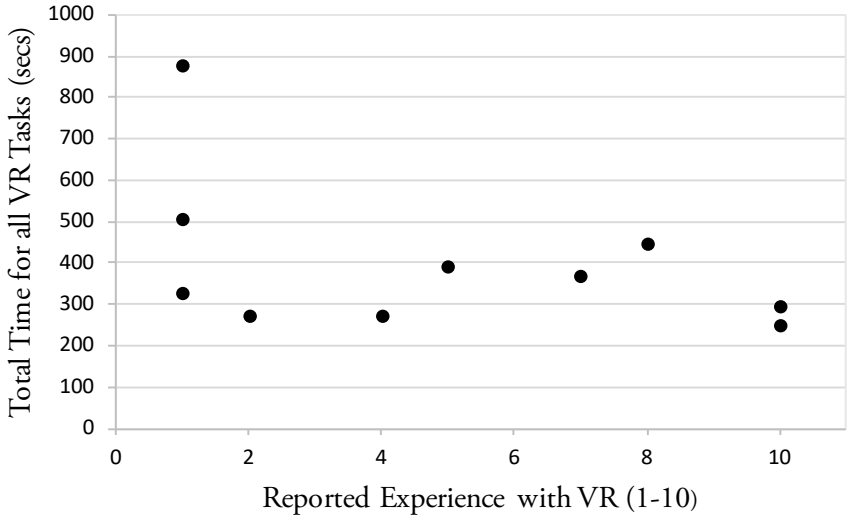

Chart 2. Time for completing VR tasks and subjective experience with VR

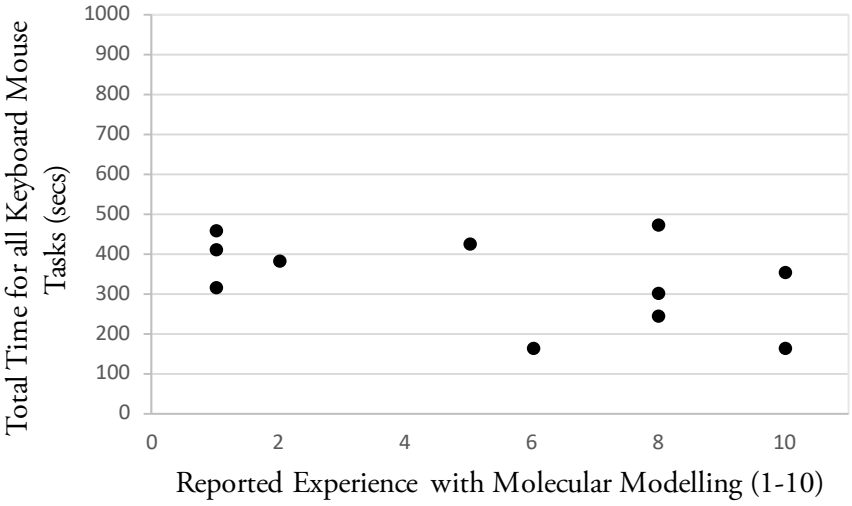

Chart 3. Time for completing keyboard and mouse tasks and subjective experience with Molecular Modelling

4.2 Results

The results of the test as recorded by the program itself are given in *Table 1*.

The next step was to review the results from the test and note the answers from the questionnaires. By doing so, we can analyse the data in a few different ways. The first is to form an aggregated score. The averaged results are given in *Table 2*.

There is a general expectation that those with more self-reported experience with VR environments would be more adept at using the new interface and take less times for completing the tasks. *Chart 2* plots the time taken by each participant for all VR tasks against their reported experience with VR devices. The results showed that those with more experience do match or outperform those with less experience. However, the more relevant observation is that there is a lot of variation within those with less self-reported experience. Most are able to learn the new interface with ease while a few struggle or fail completely.

There is also an expectation that those with experience in molecular modelling would perform better than others using the traditional interface. *Chart 3* plots the time taken for all the keyboard and mouse tasks against the participants' self-reported experience with molecular modelling software. This expectation also holds some ground but even those with no experience were perfectly capable of performing the tasks with little to no trouble.

As the data is limited and the sample size is small, further tests are definitely required and will be conducted with future versions of the prototype. It is also clear that many people in our study are competent with VR and 3D input devices already. The sample is not representative of a wide audience but does reasonably represent the target group that may use a molecular modelling program or similar programs with similar user interfaces. Computer literacy in these groups can be taken for granted but VR literacy is still growing.

Apart from these observations, there were several points that were raised through the written and verbal feedback. Some of them are expounded below.

One participant was completely unable to grasp the VR interface and abandoned the test. This was primarily because she was left handed and struggled with the heavily right-hand favoured interface. This seemed to be a less pressing issue in the development phase and there was no priority to making a left-hand option. It became a glaring shortcoming in the testing phase. There might be

some people that have less difficulty using either hand for many tasks, especially new tasks that are being learned. Others can be strongly left or right handed and a well designed user interface should either have an even distribution of hand actions or allow the user to swap the handedness. In fact, it is easier to do with 3D interfaces than with the keyboard and mouse because there are no fixed standards and no physical objects such as a keyboard that hampers the flexibility of changing the interaction method.

Another issue that varies across individuals is the depth perception or lack thereof inside the VR headset. Some people cannot see clearly without their glasses and it is difficult to adjust the lenses inside the VR display. While it is possible to wear glasses (spectacles) under the VR head mounted display, it is uncomfortable and does not always correct the issue. Other times, the problem occurs even for those who have no other eyesight problems. This may be a limitation of the hardware itself but it affects some people more obviously than others. In our tests, the simple action of selecting bonds or pressing virtual buttons was more difficult because the user would reach out too far or not far enough. In a physical interface, it would be impossible to reach too far because the interface would be in the way. And it would be clear that you have not reached far enough if there is no tactile feedback. However with virtual buttons, depth perception is key. With such large variance between the users in a group so small, it is a great limiting factor for a widely usable interface. And this variance is wholly apart from individual expertise or practice in VR environments and depends on quality of eyesight and the hardware itself to some degree. If there is some way to accommodate for people who need glasses, it would greatly improve the usability for VR devices.

The next problem which became apparent even during development was the inconsistent hand gesture recognition. In most cases, it was simply a matter of practice but it did expose that different people use their hands in different ways and it takes time to adjust to a hand gesture based input method.

Often the user tries to replace an existing atom but misses the hitbox and as a result creates a new atom. If auto-saturation is also turned on, this could result in creating multiple new unwanted atoms and bonds. The interface could be improved by increasing the size of the hitboxes and colliders for the atoms and bonds. Visual cues can also indicate when contact is made.

The biggest drawback in the keyboard and mouse interface of VR-CHEM was that users have to remember which keys to hold down. The initial design avoids on-screen handles that control movement and rotation because it requires the user to select a small hitbox in order to manipulate the target. It would be faster to hold down a keyboard shortcut. In some ways this still applies but the visual guides serve another purpose for new users by indicating what actions can be performed rather than requiring them to remember the shortcut. Those who use any program over time learn to use these shortcuts but without a visual guide for new users, there is a steeper learning curve and it might be discouraging to all but the most dedicated.

In the tests, the other students who have developed VR games could state quite clearly that the controllers in the HTC Vive were significantly better than hand gestures at handling user input in a reliable way. However the ones who spent more time with the prototype after the test ended said that once their hands adapted to the gestures that are recognised, the difference was less significant.

A weakness of the Leap sensor was in detecting subtle wrist rotations. When people interact with real objects in daily life, their hands move in intricate ways that most do not even notice because they are so used to it. Their fingers are able to grip and adjust objects in conjunction with the wrist and forearm rotation. While the sensor can detect some simple gestures it cannot see the small forces that fingers apply on the things they are interacting with. In fact, it is not only whether or not they are touching the object, but also how lightly or forcefully they press on its surface. It matters whether the fingers just graze over it to feel the texture, or if they press hard to move or deform the object. These forces are imperceptible to the sensors and limit the effectiveness of interacting with virtual objects.

The feedback from non-chemistry students also suggested that a VR environment is good for learning about molecular structures. One person commented that if this was available in his school he would have been more eager to learn about chemistry. Some chemistry students also agreed that it is a great visualisation tool even if the manipulation side was not as convenient as a simple keyboard mouse interface. Earlier such projects have focused on the visualisation aspect and this prototype was made to test if more interaction could be introduced. It seems to still be a work in progress.

5
Conclusion

The development and testing processes have been valuable learning experiences. In the conclusion, a few of the most important points are outlined. There are also some suggestions for how certain aspects of the program can be improved in the future.

The first point is about the main drawback of 3D interfaces. The initial research suggested that most current VR implementations for molecular modelling have been more effective at visualisation than at creation and manipulation. This has been the case for almost two decades and this thesis is simply a small step to overcome this limitation. The pressing issue is the lack of precision and accuracy. In the user tests, whether the participants enjoyed the VR interface or not, they largely described the keyboard and mouse to be more precise and accurate. While advanced controls for space-robots may have robust input devices, free-floating hands or hand-held controllers are not efficient for interacting with invisible virtual objects that provide no haptic feedback, resistance, or leverage. This may be sufficient for games and casual experiences, but professional scientists and engineers will prefer a more reliable interface even if the novelty of virtual reality appeals to them initially.

The next point is about the tools available for developing VR applications. Games are well supported in this area because game engines like Unity and Unreal Engine have integrated VR support. There are plug-ins, prefabs, and blueprints that are provided for easy implementation. Unfortunately, there are fewer tools for designing UI layouts and solutions for how they are positioned in 3D space. While the display resolutions are improving, they are poor for rendering crisp text that most users are accustomed to on high resolution laptop or smartphone screens. This has been an issue from the advent of VR technology (Bell & Folgler, 1995). Thus, most UI elements must be large to be legible, which leads to a lack of screen real-estate even with such a wide field of view. Developing professional programs with elaborate options and tools is more challenging than most casual games which have limited controls. This, combined with a lack of reliable feedback from virtual buttons, leads users to enjoy the experience but hardly be productive.

Mixed-reality may solve several of these issues by offering the ability to use regular input devices while visualising virtual objects. It also allows the user to glance at a regular screen or even paper for reading bodies of text and using the device to render dynamic 3D elements that respond to head movement.

The user test has shed some light on things that were overlooked in the first development phase and that information will greatly aid in the next steps of this project. The overall outcome of this thesis is a starting point for understanding the user interface demands of professional programs. Hopefully, future work will find solutions for most of the current limitations.

Appendix

User Test Questionnaire

Name (optional):

Age:

Field of study:

Questions- Rate from 1-10 (1 being strongly disagree, and 10 being strongly agree)

Q1. I have prior experience with VR. ( )

Q2. I have prior experience with molecular modelling. ( )

Q3. I find 3D user interfaces more *intuitive* than keyboard + mouse. ( )

Q4. I find 3D user interfaces more *convenient* than keyboard + mouse. ( )

Q5. I find VR more *immersive* than 3D models on a regular screen. ( )

Q6. I feel *uncomfortable* using VR devices. ( )

Q7. I understood the tasks that I was asked to perform in VR-CHEM. ( )

Q8. VR-CHEM has an *intuitive* interface in the VR mode. ( )

Q9. VR-CHEM has an *accurate and precise* interface in the VR mode. ( )

Q10. VR-CHEM has an *enjoyable* interface in the VR mode. ( )

Q11. VR-CHEM has an *intuitive* interface in the keyboard + mouse mode. ( )

Q12. VR-CHEM has an *accurate and precise* interface in the keyboard +mouse mode. ( )

Q13. VR-CHEM has an *enjoyable* interface in the keyboard + mouse mode. ( )

Questions- brief answers

Q14. What would you improve in the VR-CHEM interface?

Q15. Would you use this in your work if it were a full featured product? Why or why not?

Q16. What additional features would you want to see in the future of VR-CHEM?

Questionnaire Responses

This table gives the responses that participants wrote in their questionnaire for the questions requiring a number between 1 and 10 as an answer.

Tester	Q1	Q2	Q3	Q4	Q5	Q6	Q7	Q8	Q9	Q10	Q11	Q12	Q13
1	8	5	10	5	0	1	10	10	7	10	8	7	8
2	1	10	8	3	8	2	10	9	7	9	9	9	8
3	1	8	8	7	8	9	10	9	2	10	8	9	9
4	5	10	9	2	10	1	10	8	3	10	8	8	9
5	2	8	6	5	8	6	9	6	4	5	5	8	7
6	1	8	4	6	9	1	9	9	8	9	7	8	7
7	7	6	7	6	9	3	10	7	7	8	8	9	6
8	1	2	2	5	5	7	10	5	5	5	5	5	7
9	10	1	8	6	10	9[sic]	10	7	7	7	3	5	5
10	10	1	6	8	10	1	10	9	9	10	8	9	8
11	4	1	7	6	7	7	8	6	5	7	6	7	5

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