

Mixed Reality for Visualizing the Structure of Organic Compounds using Microsoft HoloLens - A Review

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Abstract - Education is the foundation for a flourishing society and the process of passing on information and knowledge has always been a prime concern. People are constantly looking for ways to make knowledge transfer more easy, quick, and efficient. In this era of digital devices, Mixed Reality paves a new way for delivering educational content, thus being effectively used to strengthen students' understanding and engagement. The objective of this paper was to propose the design of a system that helps visualize the structure of various organic compounds. The proposed approach helped students better understand and compare different hydrocarbons and their respective structures. Transformations like Scale, Rotate and Translate provided a detailed aspect of each compound. An attempt has been made to overcome traditional 2D learning problems relating to perspective and cognition by using 3D models and adding various interactions in the Mixed Reality environment with the help of Vuforia markers and HoloLens, which together have a strong influence on developing meaningful learning. The use of interactive visualization through multi-dimensional graphics and simulation can provide an opportunity to present key learning content for students.

Key Words: Mixed Reality, Microsoft HoloLens, Organic Compounds, Vuforia, Education

1. INTRODUCTION

The value of traditional learning approaches in system modelling has been challenged with regards to students' understanding, learning performance and mastering of modelling techniques. The traditional way of visualizing certain concepts on a 2D screen may not be intuitive anymore, but we can always gain new depth of knowledge by visualizing them in a 3D environment. Organic chemistry is the study of structure, properties, composition of carbon-containing compounds (including hydrocarbons). It is an area that is perceived as difficult to understand, because it requires three-dimensional thinking. Some of the problems faced by students while learning organic chemistry is the inability to see and manipulate three-dimensional structures on paper. Mostly these are problems that relate to cognition and the process

of learning. Imparting knowledge with the help of pictures/videos or through traditional print textbook does not (present abstract concepts as tangible objects that can be manipulates) promote authentic engagement of students. Using a 3D approach improves spatial awareness and thinking in STEM subjects to a great extent.

The Reality Virtuality Continuum was introduced by Paul Milgram [1]. It is a continuous scale ranging from completely real reality to completely Virtual Virtuality and encompasses all possible variations of real and virtual objects. Fig. 1. Shows the continuum which to its extreme left has the Completely Real Environment - The physical space we live in, where real objects are overlaid on a real environment. Moving on, we have Augmented Reality - Virtual objects being overlaid on a real environment. Next up is Augmented Virtuality - Real objects being overlaid on a virtual environment. Finally, we have the Completely Virtual Environment - Virtual objects are overlaid on a virtual environment. The area between the two extremes where the real and virtual environments are mixed is termed as Mixed Reality - Virtual objects being overlaid on a real environment in addition to direct interaction with these objects.

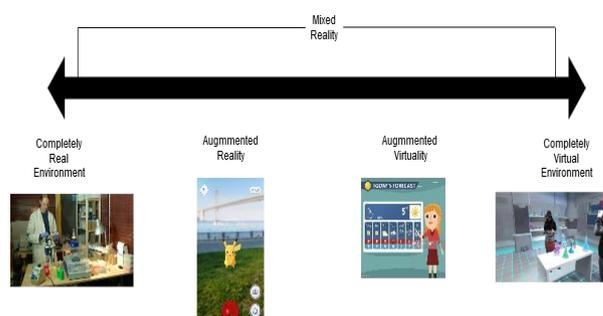


Fig -1: Reality Virtuality Continuum

The immersive technologies that are acquiring momentum are:

Augmented Reality (AR), Virtual Reality (VR), Mixed Reality (MR).

- **Augmented Reality:**

AR permits the user to perceive the real world, with virtual entities superimposed upon or composited with the real world [2]. Here, the virtual (computer-generated) objects appear to coexist in the same space as the real world [3]. AR systems track the position and orientation of the user's head so that the overlaid material can be aligned with the user's view of the world [4]. It generates stimuli at real time for the user's interaction that are superposed over the physical environment of the user [5]. An AR system includes a camera able to track the user movement for merging the virtual objects, and a visual display, like glasses through that the user can see the virtual objects overlaying to the physical world, adequate processing power for graphics and animation [6]. Augmented Reality, unlike Virtual Reality, does not seek to withdraw the user from the real environment; rather, it brings virtual elements that integrate into a physical space [2].

- **Virtual Reality:**

In the case of VR, the real world is replaced by virtual objects and scenarios. It completely replaces what we have come to consider normal reality. Since a person is completely immersed in the virtual environment, he has no awareness about his/her surroundings. It produces an appearing of reality that allows the user to perceive a sensation of presence inside of it [5].

- **Mixed Reality:**

MR is an amalgamation of physical objects and virtual objects/components that are overlaid onto the physical world. These virtual objects can be interacted with. Rather than being superimposed on top of normal reality, as is done with augmented reality, MR experience blends the two realities together to create a new mixed reality. MR not only allows user's interaction with virtual environments even allows physical objects from the immediate environment of the user to be elements to interact with the virtual environment [5]. It is basically as continuum of the previously mentioned innovative technologies, provides a framework to position real and virtual worlds [7]. The benefit of our approach of implementing Mixed Reality in our project is that it promotes the potential to interact with the 3D structures and with the real world in the same context and

time frame which comes handy when it comes to perform comparison between 3D hydrocarbon structures.

The motive of our application is to study the structure of Organic Compounds using Microsoft HoloLens. It is a Mixed Reality app that gives you the ability to visualize and interact with various hydrocarbons thereby changing over the current approach to education i.e., traditional teaching methods that are focused on providing facts, however having access to and consuming a lot of information that does not contribute to authentic learning. A lot of people have difficulties comprehending information. Using MR, students can be provided with easy demonstrations of crucial concepts through interactive experiences. Thus, through our application, we aim towards creating an interactive 3D environment that effectively simulates visualization of hydrocarbons along with a detailed description of each. The major difficulty in understanding the concepts of Organic Chemistry is that it has a requirement of stereoscopic visualization to get the understanding of compound structures [8]. Students find learning chemistry in real space exciting and with the 3D model being interactive, they can remember the structure vividly. Our application provides a student abundant space to perform comparisons between the chemical structures, which aids them to clear their chief doubts. Results from a few researches show improvements in student performance after using 3-dimensional learning methods. It is necessary that these methods are used frequently which in turn is beneficial to students for long term retention.

Following is the way the remaining paper is organized:

Section 2 includes the literature survey, Section 3 gives a detailed description of the adopted methodology for the proposed system, and Section 4 draws conclusion and future work.

2. LITERATURE REVIEW

The process of gaining knowledge through experience or feedback is termed as experiential learning, contrary to lectures and classroom learning. During the process of learning, the learner is in touch with the realities of what is being studied. Kolb's Experiential Learning Theory (ELT) integrates a framework that aims at addressing 21st century issues of learning and education. Through ELT, the aim is to explain how experience is revolutionized into learning and reliable knowledge [9]. Technologies part of the Reality-Virtuality continuum provide a simulated environment which gives users an immersive experience, thereby enabling learning by being in touch with the concept's reality. Conrad Tucker, a professor, believes that replacing traditional learning methods with immersive experiences will enhance education. He observes that currently, there aren't many online courses related to

STEM. These are some of the domains, especially Engineering, that always have the need of laboratories. While incomes are continuing to remain steady, the cost of education is soaring. Augmented, Virtual and Mixed Reality can be a helping hand in reversing the cost curve [10].

Supporting education with 3-D instructions is bringing a whole new dynamic to classrooms. A systematic review was conducted to test the efficacy of VR based teaching on students. The study analyses to see if advantages of the technology helped students in retaining information and favorable results were achieved, thus showing that the effects of VR learning provided better retention irrespective of when the assessment was carried out [11]. Such technologies provide the right set of circumstances that help in engaging students. Incorporating Virtual Reality into higher education curriculum impels students to learn and escalates their engagement. Students can immerse themselves into a virtual environment that delivers a whole new platform by providing them with the information they need and an interactive experience [12]. Virtual reality has allowed creation and simulation of numerous situations of information presentation (e.g., a virtual museum), object manipulation (e.g., a virtual anatomy laboratory) as well as problem solving, which permits its wide use in Education [13], [14], [15].

Students who possess spatial ability can surely delineate a spatial object even when the spatial entity isn't in front of them. With the help of spatial cognitive skills, a person learns to imagine, and inwardly represent real world objects from different perspectives [16]. Spatial potential consists of spatial visualization, spatial orientation, and spatial relations [17]. Spatial visualization basically encompasses the mental representation of a spatial entity as well as performing manipulation over these spatial 3D objects. Spatial orientation refers to the capability of a person to be able to envision the pose and direction of an entity. It can be achieved by performing transformations on the object. Spatial relations are the ability to form mental relationships between objects [18]. Through representation, a person's abstract mind can be known. Hence representation of abstract concepts is principal in the field of education. Spatial abilities are one of the cognitive factors that are relevant to the mastery of chemistry concepts because it includes various scenarios where a 3D mental model of a 2D depiction must be assumed and possibly mentally rotating it, e.g. To know the bond angles [19]. High spatial ability students generally perform better in chemistry because they are able to mentally manipulate data belonging to spatial domain or represent complex information visually. [19]. Students are expected to translate a chemical formula into its molecular structure(s), visualize the corresponding three-dimensional (3D) configurations, and compare these configurations. Therefore, being able to comprehend and mentally manipulate chemical representations is critical for students to understand the content and conduct advanced scientific research.[19].

Creating fine 3D content for chemistry education has exhibited great improvement in grasping and visualizing compound structures. A demonstration of the application of AR in classrooms and laboratories is done using a smartphone application and notecards. The instructor can create required AR content which can eventually be accessed by students upon downloading the application. Feedback given by the students included an ease in understanding the taught concept and an illusion that the user is walking through the setup process in the laboratory [20].

3. METHODOLOGY

A. Elements of the application:

- Microsoft HoloLens:
Microsoft HoloLens is a mixed reality (MR) device that permits the user to engage and interact with digital 3D content and collaborate with both real-world artefacts and virtual artefacts in the form of holographic-like images [21]. It is a head-mounted device comprising of multiple and diverse sensors, a computer, and a stereo pair of display panels. The built-in sensors include four cameras on the sides, a video camera at the front, a depth camera, and an inertial measurement unit (IMU). The computer includes a custom-built Holographic Processing Unit (HPU) with 2GB RAM designed for fast processing of holograms [22]. Important HoloLens features that have been used in the application:
 - Gaze: Gaze is the first mode of input and discloses and aids the user's intent and awareness [23].
 - Gesture: Gestures convert user intent or motive into some action. With gestures, users can interact and play around with holograms. It tracks the user's hand's position, acknowledges, and responds to user input, and give feedback to the user established from hand state and position [23].
 - Spatial mapping: The spatial mapping feature of HoloLens grants real-time display of the constructed 3D mesh on the stereo display panels of HoloLens creating a mixed reality visualization of the map [22]. Microsoft researchers have previously developed Kinect Fusion [24] which is a simultaneous localization and mapping (SLAM) algorithm for real-time 3D scene reconstruction and the same is being used here as well.

Fig 2. shows the Microsoft HoloLens 1st Gen



Fig -2: Microsoft HoloLens

- **Holograms:**
HoloLens lets you create holograms, which are 3D graphical models [22] made of light and sound that appear in the real space around you, just as if they were real entities. These holograms can be interacted with, with the help of gaze, gestures, and voice commands, and these can also collaborate with real-world surfaces around you. With holograms, you can create digital bodies that are ingredients of real world. Fig.3. shows a sample hologram.

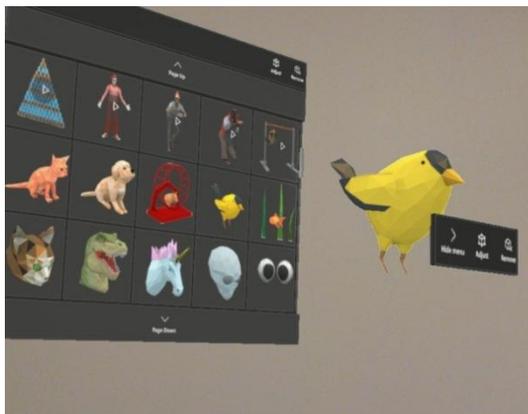


Fig -3: Sample Hologram

- **Unity engine:**
Unity3D is one of the most famous virtual reality and mixed reality tools that has windows mixed reality and HoloLens support, also a cross-platform game development software, and besides Mac OSX, Unity3D can fully support Windows XP/Vista/7, Unity3D supports three scripting languages: JavaScript, C#, and a dialect of Python called Boo [25]. It provides rich functionalities to create and deal with Holograms.
- **Vuforia:**
The Vuforia engine allows us to use Vuforia Image Targets to recognize an image and augment it with digital 3D content rendered on Microsoft HoloLens.

- **Visual Studio:**
The final solution file (.sln) gets compiled here and the app is deployed on the HoloLens.
- **Mixed Reality Toolkit:**
The Mixed Reality Toolkit (MRTK) is a cross-platform toolkit comprising of packages and resources used for building Mixed Reality applications.

Important features:

- **Camera system**
The camera system enables the Microsoft Mixed Reality Toolkit to configure and optimize the application's camera for use in mixed reality applications.
- **Input system**
MRTK's Input System provides elements like interact-able object, cursor, focus and pointers which are crucial for input management.

B. Proposed System Architecture:

The elementary organization of the system, embodying key elements, their relationships to each other and to the environment is covered here.

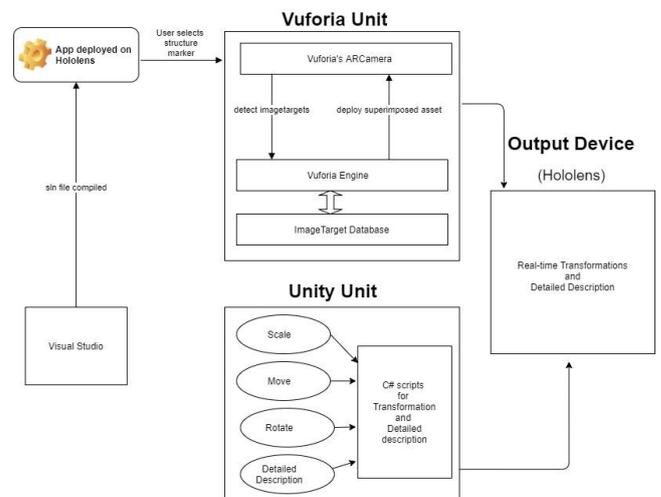


Fig -4: Proposed System Architecture

Fig. 4 shows the system architecture which has 4 main units as follows:

- **Visual Studio Unit** - The final solution file (.sln) gets compiled through and the app is deployed on the HoloLens.
- **Vuforia Unit** - Its AR camera detects the image target, interacts with the Vuforia Engine which in turn reaches out to the Image Target Database to provide the corresponding 3D asset that needs to be superimposed.

- Unity Unit - Maps hand gestures for transformations and enables the corresponding C# scripts.
- Device Unit - Application is deployed and 3D structures are visualized.

Image Targets are images which will be identified by Vuforia's SDK and what sets apart these image targets from QR codes or data matrices is that they don't require special black and white regions or codes to be detected. These image targets are recognized based on features naturally present in the image. Once detected, Vuforia will track the image along the camera's field of view. A sample image target is shown in Fig. 5.



Fig -5: Sample Image Target

Post detecting an image target, its corresponding 3D model needs to be superimposed on it. One such 3D model of the compound Methane is shown in Fig. 6.

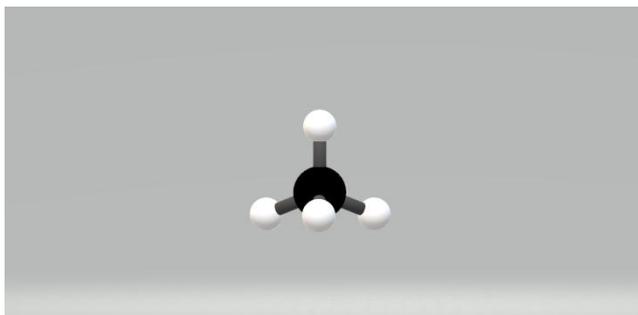


Fig -6: Methane Model

The detailed process, as envisioned, right from defining the image target to associating a 3D model with it is depicted in Fig. 7.

For image target recognition and rendering you need to define your image target on which you want to superimpose your 3D object. On the Vuforia developer console, we create a custom database into which we put our target image. Every image uploaded onto the target manager will have a star rating associated with it which denotes the number of features present in the uploaded image. Higher the star rating, more the features. This image now has to be brought into the unity environment. But firstly, to implement Vuforia in our

project we have to specify the key in our project which is available on the Vuforia developer console. In Vuforia settings, we then import our database which holds our target image. In the next step the appropriate 3D model needs to be created which will be superimposed on a particular image target. This model can be created in any 3D model creation tool like Blender which then has to be imported into Unity in fbx format. Finally, the model will be added as a child (every scene in unity follows a hierarchy) of the image target.

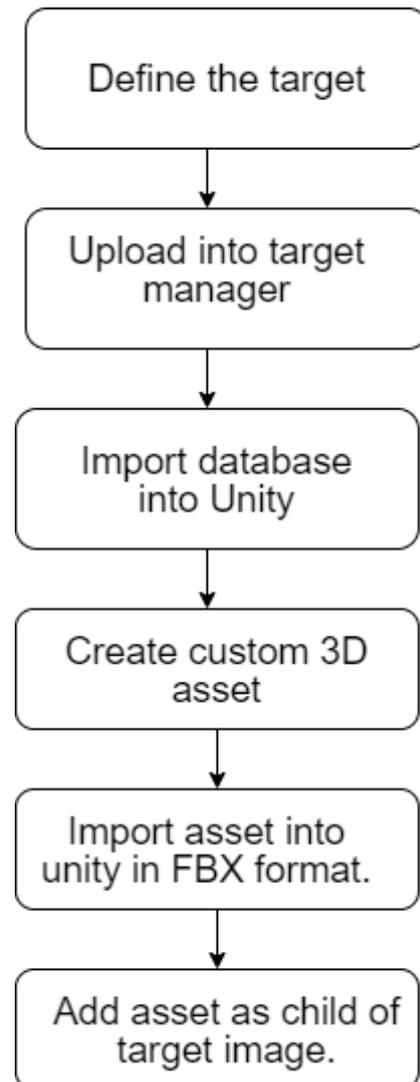
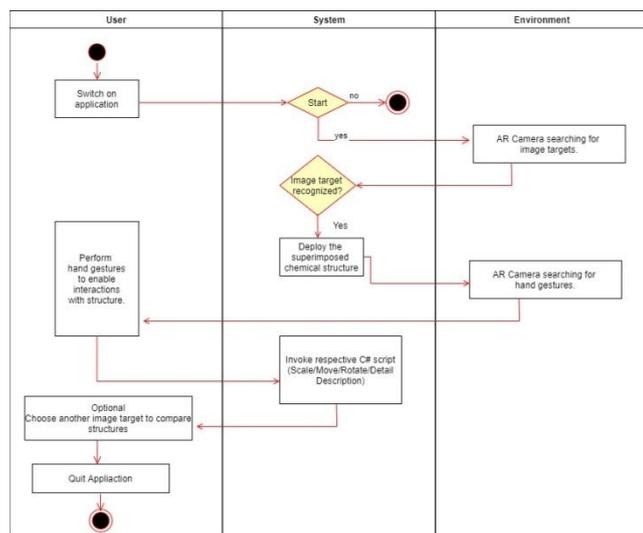


Fig -7: Vuforia Image Target Process

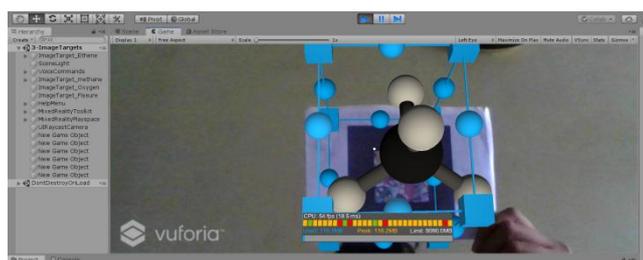
C. Proposed Working of the Application:

Fig 8. illustrates the expected working of our application.


Fig -8: Expected Working

When the application has been deployed and started, the HoloLens' Mixed Reality camera (with Vuforia ARCamera support) will start searching the physical space to detect any image targets. The user selects a structure marker, which when detected by the camera, its corresponding 3D model structure is rendered by the Vuforia engine and deployed on the HoloLens, which is seen by the user. To perform transformations like rotate, scale and translate, hand gestures will be performed by the user which when recognized, the unity engine will enable required C# scripts and changes will be observed. The HoloLens and Unity Engine map these gestures and enable corresponding C# scripts.

Using unity editor, the proposed model was validated for a basic hydrocarbon - methane which resulted in the output shown in Fig. 9.


Fig -9: Sample Output

The 3D model of methane is enclosed by a Bounding Box which has cubes and spheres on each of its sides. Using the cube and sphere, scale and rotate transformations can be applied on the model respectively.

4. CONCLUSION AND FUTURE SCOPE

In this project, we propose a Mixed Reality application to visualize the complex structures of molecular compounds in Organic Chemistry using image targets, effectively reducing the complexities to visualize chemical structures

and properties in 3D space. Once the structure is visualized on the HoloLens the students can then play around with the structure thus increasing the learnability. Outcomes are expected to be an overall improvement in final skill level for all students. Considering the fact that mixed reality is a culmination of physical world and the virtual objects we don't have the restriction of a physical space/environment which can be used to our advantage. Students can rearrange multiple 3D structures to make comparisons which helps in better understanding of the compound family i.e. Alkane, Alkene, Alkyne, thus increasing the workload of our application.

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