Chemistry Laboratory in Virtual Reality for Immersive Learning Experiences

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ABSTRACT
Traditional chemistry classes are usually lacking, when it comes to a student's need to learn in-depth about the practical side of this subject. Due to the cost, shortage of necessary equipment, the lack of safety measures for certain chemical reactions, and the number of students, chemistry experiments are rarely done in schools and are often conducted by teachers. VR technology can be utilized to surpass the challenges faced by conventional ways of teaching chemistry, by providing immersive virtual environments where students can learn. VemClass an educational application where students can practice the theoretical notions accumulated during chemistry lessons, is presented in this paper to analyze whether VR technology has the potential to improve the learning process and to transform the ways in which students engage during classes, cultivating a deeper knowledge and increasing the level of enjoyment for this subject.

Author Keywords
Virtual Reality; Chemistry Laboratory Simulation; Obi Fluid; Educational Application; Immersive Application

ACM Classification Keywords
Human-centered computing: Human computer interaction (HCI); Interaction paradigms; Virtual reality

General Terms
Virtual reality; Particle-based liquid simulation; Input devices; Head-mounted display

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INTRODUCTION

Virtual reality (VR) and augmented reality (AR) are emerging technologies that are rapidly rising in popularity across various industries. With the possibility to revolutionize the way we interact with digital information, the most notable fields in which VR and AR are proving their usability include but are not limited to health care, education, engineering design, manufacturing, retail, and entertainment [1].

The announcements of two new mixed reality (MR) and VR headsets, being launched by Apple and Meta [2], show that AR and VR are subjects of interest for big tech companies that are aiming to improve the current technology.

In the educational field, VR can downright change the way students comprehend theoretical ideas and are trained for the practical aspects of every discipline. Schools can benefit from immersive technology as keeping students active during classes and encouraging them to be curious is one of their goals. VR and AR technology is expected to become more cost-effective and reliable, given tech giants, such as Facebook, Google, and Apple are supporting the growth of this type of technology [3], [4]. Therefore, educational institutions might consider investing in VR and AR technology, at some point in the future.

VemClass is an immersive educational application, where a chemistry laboratory class is simulated in VR, which should assist students in learning about the practical aspects of chemistry. This application has simulated chemistry experiments that are targeted to teach students from middle school and provides the possibility to directly interact with various chemistry objects in the virtual environment using hand presence. The application is intended to run on a VR headset, such as Meta Quest 2, to experience an immersive first-person view, while also using the hand controllers to simulate hand interactions. Students that utilize VemClass have as their objective the completion of the chosen experiment, by following the instructions given by the application. The experiment simulation uses an advanced particle-based physics engine capable of rendering liquid behavior, and other details such as liquid diffusion, foam, and bubbles. The students can interact with the environment by grabbing objects and triggering them to perform tasks, such as a pipette pouring liquid. VemClass also has additional features such as visualizing a video to better understand the experiment's required steps, written instructions, writing on the whiteboard and teleportation in the scene.

The most important advantage of VR technology stands in the emotional response coming from the students who are utilizing it. Traditional lessons are often perceived as monotonous, uninteresting, and difficult to follow, whereas engaging VR environments can improve the learning process by giving an amount of novelty in class. Students' level of motivation is increased, and so is their attention span, resulting overall in better learning performance [4]. Another advantage of virtual reality is that it can allow for experimenting in those situations that are otherwise not accessible physically, such as time problems, dangerous situations, or ethical problems [5]. In our case, students following experiments in traditional chemistry laboratories are at risk, given the possibility of injury coming from the reactions between chemical compounds or the usage of harmful chemicals.

The conclusions that are drawn from the development of this immersive application can contribute to the field of educational technology. VemClass application can stand as a starting point for the development of future VR applications for chemistry and encourage improvements in technology-enhanced teaching across a range of subjects.

RELATED WORK

Immersive vs Non-Immersive Applications for Learning

As Freina noted [5], for virtual reality, the term "immersion" refers to the sense of being physically present in a virtual environment, this perception being created by visuals, sounds, or other stimuli so that the user feels immersed in the simulated world. Non-immersive virtual reality also exists, and it refers to a user placed in a 3D environment that is displayed and manipulated by conventional technology, for instance, a monitor, a keyboard, and a mouse, therefore the user does not feel immersed in the virtual world.

As Makransky concluded in the article [4], compared to non-immersive technologies such as desktop VR simulations, immersive VR has been preferred, as it is better at arousing, engaging, and motivating students. Also, it provides a greater sense of control and autonomy in the learning process, due to head-motion tracking. Students who are motivated have been shown to set higher educational goals, learn deeply and have higher academic achievements. Although, the increase in motivation and other positive results might be due to the novelty of the technology [4], [6].

Immersive VR in Education

Elmqaddem argued, in its paper [3], on whether VR and AR technologies have evolved enough in the last years to meet the needs of the 21st-century learner. This technology has been improved not only regarding hardware but also software, by big tech giants such as Google, Facebook, HTC and Sony, and it is still in exploration regarding its usage in various fields, including education. The possibility to manipulate objects in the scene, with the usage of controllers, is considered in the paper to be an important step towards utilizing VR for learning, allowing students to practice by interacting with virtual objects. The author concludes that AR and VR technology will find its place in future education, as it is expected to become more accessible and reliable.

As stated by Freina in the survey on the literature on the potential of using Immersive VR in Education [5], many papers refer to university and pre-university teaching, the attention being focused mostly on scientific subjects, such as chemistry [6]. The verdicts drawn were that VR can offer great benefits for learning, by offering a safe environment for exploration and by raising the motivation for learning, due to the game-like approach. The author continues to conclude that starting from middle school VR can give advantages, by allowing direct interaction with objects or situations that are physically out of reach, helping to improve learning and memorization.

Chung-Ho Su noted in his study [7] the educational achievements that students can have after utilizing a VR chemistry laboratory simulation. A VR chemistry laboratory has been designed and developed for the purpose of this study. The author noted the importance of concrete experience as stated in Kolb's learning cycle, and that VR chemistry laboratories allow students to transform their practical experience into knowledge. The conclusion was that virtual reality laboratories have the potential to increase student's motivation to learn and, in the end, raise their academic achievements.

Dunnagan's article [8] also focuses on the impact VR can have on chemistry education as opposed to traditional laboratory sessions. The study shows that there are minimal differences between the VR approach and the traditional laboratory experimentation, stating that for the students who are unable to attend lab, VR technology can represent a suitable replacement. The study argues that not all laboratory sessions should be replaced with a simulation, instead, VR should be used as an alternative method when physical experimentation is not possible.

Current Applications

ClassVR [9] is a product made by Avantis System, a leading educational technology company, that provides schools with VR technology, and lessons according to the curricula, and comes with the complete set of the necessary equipment from hardware to software. But it seems that in the case of chemistry lessons, the laboratory experiments have not yet been integrated into the software and only the molecular visualization of chemical compounds is available to students. It is also specified that VR class headsets can be gesture-controlled, but no information is given about the hand presence mechanism that would be needed to interact with the VR laboratory.

VR Lab Academy [10] provides software in which various chemistry experiments can be carried out in VR, according to the curriculum, but the necessary hardware resources are not few due to the usage of Oculus Rift VR headsets which require a VR-Ready PC. Schools might not consider this to be cost-effective, due to the necessity to buy better PCs and not only VR headsets. VR Lab Academy does not have particle-based liquid simulation; therefore, the liquid is not very realistically rendered. Also, it does not support teleportation in the scene. If physical movement is required, then it can be quite limiting depending on the boundary size. However, if movement is done by utilizing the joystick, then this can cause motion sickness. VemClass supports teleportation in the scene, and it is utilizing Obi Fluid for particle-based liquid simulation.

THEORETICAL FOUNDATION

Chemistry Curriculum

The application has educational content that respects the Romanian chemistry curriculum for 7th and 8th grade. A list of experiments is proposed in the curriculum, and it includes acid-base identification as an experiment for the 7th grade and the reaction of zinc with hydrochloric acid (HCl) as an experiment for the 8th grade. The application has simulated those enumerated experiments.

Reaction of zinc with hydrochloric acid

The reaction between HCl and Zinc is a single replacement reaction, where zinc metal displaces the hydrogen to form hydrogen gas and zinc chloride, a salt. It is an exothermic reaction and is represented by the following equation, where hydrogen gas is released:

$$Zn + 2HCl \rightarrow ZnCl_2 + H_2\uparrow$$

To recreate this reaction in a virtual environment, a fluid simulation is required to render the HCl as a liquid. Also, foam and hydrogen bubbles appear from the reaction and those need to be simulated as well, to represent hydrogen. Additionally, an even better way to highlight the presence of hydrogen is to accumulate it in a container and then set it on fire by using a lighter, as shown in Figure 1. Such an action is dangerous to be made by a student but is still a perfect way to demonstrate that the gas eliminated is hydrogen, and here is where VR proves itself to be helpful. A water pot is also used to show the presence of hydrogen bubbles, as the resulting hydrogen travels from the flask through a tube into the water pot. This is also implemented in the application.

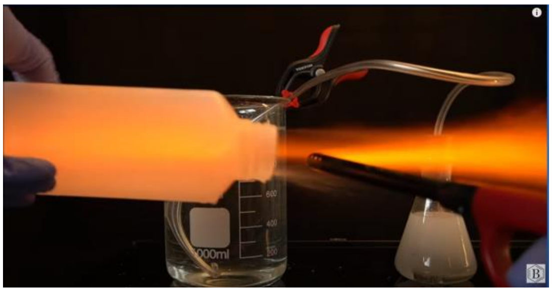

Figure 1. Burning of the hydrogen accumulated in a container.

Acid-base identification

Acid-base identification is a type of experiment that is made in the 7th grade and is utilizing some indicators to determine if a substance is an acid or base. Acid-base indicators are compounds that change color when protonated or deprotonated. These substances are often used in titration, to determine the concentration of an unknown substance, but are also used to determine pH level value and for fascinating color-change science experiments. Such indicators include phenolphthalein, methyl orange and the universal indicator solution. The indicators will change the color of the liquid depending on its pH level, for example, the methyl orange indicator will change the color of acid to red, and of a base to yellow.

Usually, the indicator solutions are lower in density, meaning they will tend to stay on top. For this experiment, a fluid simulator should be used, where it is possible to set the liquid properties such as viscosity and density. The diffusion of liquids should also be represented more realistically, instead of just changing the color of the whole liquid, the color of only the particles of the liquid that is interacting with the indicator solution. Figure 2 shows the color transition happening for acid-base identification.

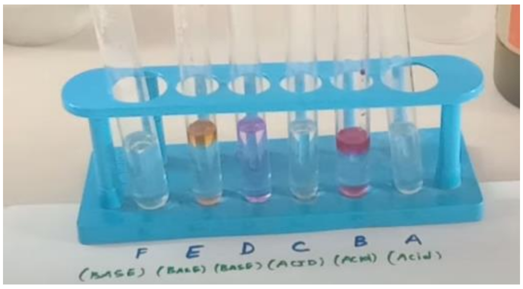

Figure 2. Liquid diffusion for acid-base identification

FLUID SIMULATION

Zibra Liquids

A modern plugin for real-time liquid simulation and rendering named Zibra Liquids [12], appeared in 2022. It takes advantage of AI for neural object representations and uses a physical solver for liquid simulation. By using AI, Zibra Liquids can offer a high-performance simulation of the interaction of liquids with objects of complex shapes. It supports VR development and is intended to be used for small to mid-scale simulations. The disadvantage is that the cost for this plugin is rather high, yet they provide a free version that is quite limited in terms of how many colliders can be used, and the shapes that are allowed. The free version might have serious drawbacks for this project, and it might not be utilizable due to its limitations. Both the free and not free 2022 versions do not support the mixing of liquids feature, which is an important aspect for this application, however, a newer version of this plugin was released in May 2023, which also supports mixing of liquids.

Obi Fluid

Obi Fluid is an advanced particle-based physics engine used for simulating liquid. It offers 3D real-time simulation of fluid and adjustable properties of fluids for surface tension, stickiness, viscosity, vorticity, and many other properties, while also supporting multiple types of colliders. It allows for diffusion of liquid which is exactly what is needed for this application, and particle advection which is necessary for generating foam and bubbles. It supports VR and is intended to be used for small-scale liquid simulations. However, to allow the liquid to be rendered by Obi Fluid the render mode should be set to multi-pass, which is a significant drawback in terms of performance. The computational power that is required for liquid simulation with Obi Fluid is substantial, and therefore, performance issues might arise if the number of particles is large, or if the resolution of the liquid is very small.

Particle diffusion is achieved with Obi Fluid by having 4 diffusion channels [13]. The diffusion channels do not have any special meaning and those can be used for color mixing, temperature diffusion or any other property. When two particles from the same solver collide with one another if the diffusion property is set at a specified rate, then the particles exchange the data from the four diffusion channels, based on the rate, until they have the same color as shown in Figure 3.

Figure 3. Particle diffusion with Obi Fluid

Particle Advection is used for simulating such as foam, smoke, and bubbles, to make the regular Unity particles passively carried out by the Obi Fluid liquid [13]. The working principle is that for every regular unity particle Obi finds the closest obi fluid particle, within a set range. Then the particle velocity will be equal to the weighted average of the velocities of the found obi fluid particles. Figure 4 shows how particle advection happens, where the red dots are unity particles, and the white dots are obi fluid particles.

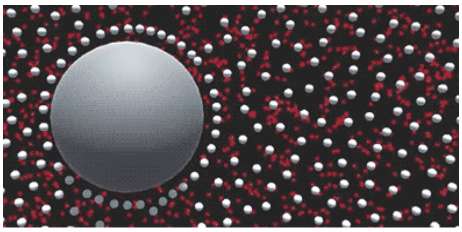

Figure 4. Particle advection with Obi Fluid

DESIGN AND IMPLEMENTATION

Tools and Plugins

The VR headset that has been used for running the application is Meta Quest 2, a popular headset that can be used as both a stand-alone device and as a headset connected to a VR-Ready PC, through Oculus Link. For the development of this application, Unity Engine has been chosen, which allows for fast development of VR applications as it provides the XR Plug-in Management, to install the desired plug-ins for VR development. OpenXR toolkit has been selected as it targets a wide range of devices, including Meta Quest 2, and many others. XR Interaction Toolkit is utilized for processing the inputs, it does support OpenXR and is utilized for performing actions such as grabbing, selecting, and hovering.

For this application, Obi Fluid particle-based simulation engine has been chosen, as it is more relevant for the type of liquid simulation that is expected to be implemented. It supports all the features that should be found in the project, such as liquid rendering, colliding with objects, color changing with diffusion, foam generation and others. However, this method is expected to have performance limitations.

Conceptual architecture

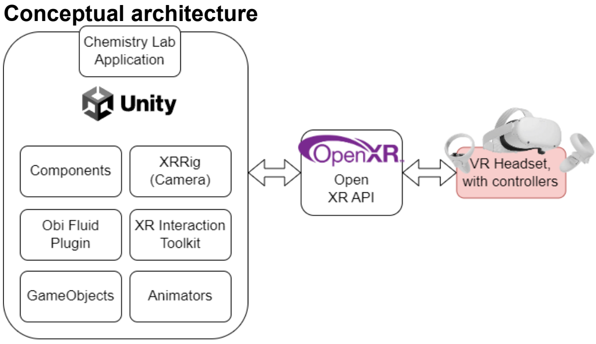

Figure 5. Conceptual architecture.

The conceptual architecture is shown in Figure 5. The application requires the usage of VR headset and controllers for interaction. OpenXR plugin is responsible for rendering the images on the headset, and for receiving the inputs that the Oculus controllers send. XRRig holds the camera and hand controllers, and this will be the object that will be manipulated by locomotion. XR Interaction Toolkit is used for processing the interaction for this application.

Use cases

The application supports the following use cases, as shown in the use case diagram, Figure 6.

Switching experiments is a use case that allows the user to choose between the available experiments.

The *Reaction of zinc with HCl experiment* is a use case where the simulated experiment can be conducted. The user can pour HCl and drop zinc granules in a flask. Hydrogen bubbles can also be seen in a water pot, after moving through the connected tube that the user must attach. Finally, the user can also burn the hydrogen resulting from the reaction that was accumulated in a container.

The *Acid-base identification experiment* is another use case where an experiment is simulated. This time the user can determine if a solution is an acid or base, by pouring the indicator solution in the tubes.

Writing on the whiteboard is a use case that allows the user to write something on the whiteboard.

Playing educational video and *Showing instructions* are use cases that have to role in informing the user about the experiment's purpose and providing guidance for performing the steps.

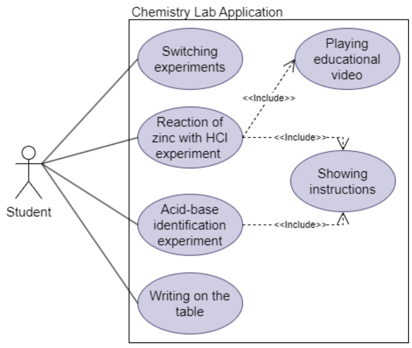

Figure 6. Use case diagram.

Project structure

The project will have the following structure shown in Figure 7.

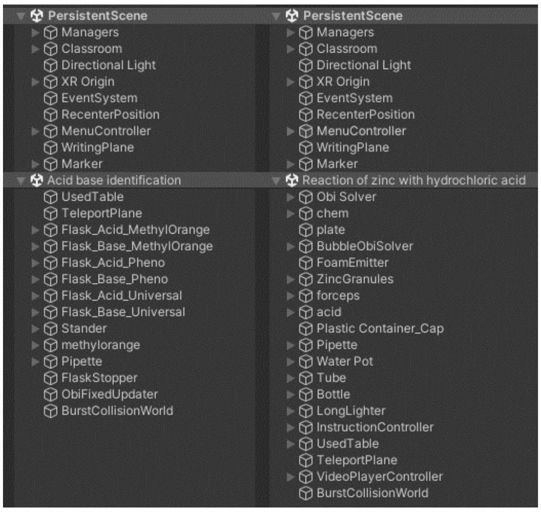

Figure 7. Project structure.

The *Persistent Scene* is the primary scene. The experiment scenes, which are the *Acid base identification* scene and the *Reaction of zinc with hydrochloric acid* scene get loaded additively on top of the primary scene.

Scene loading

The project has a scene for each experiment holding all the GameObjects that are related to that experiment, to avoid a big, bloated scene, that is difficult to maintain, where all the GameObjects in the application are placed. Additionally, there will be multiple objects that are going to be present in the application from start to finish and are not dependent on the current experiment that is being shown. Those objects should not be replicated across the scenes that belong to each experiment, as it will be very difficult to maintain, and instead placed in the *Persistent Scene*. The *Default Scene* is loaded at the application start, being the scene where the menu for selecting experiments is shown. Figure 8 illustrates the idea of loading the secondary scenes for the experiments, on top of the *Persistent Scene*.

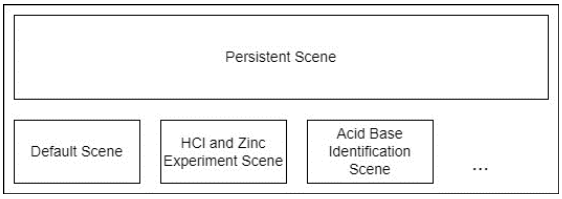

Figure 8. Scene loading method.

Reaction of zinc with HCl experiment

For this experiment liquid pouring is needed. To implement liquid pouring with Obi Fluid it is needed to set up an Obi Solver and Obi Emitter. A pipette object will be used to pour the liquid, that needs to be filled, from an HCl bottle. With Obi Fluid various properties can be set for a fluid blueprint, with the most important being resolution, capacity, density, smoothing, viscosity, and surface tension. Figure 9 shows the properties that have been set to simulate the HCl liquid.

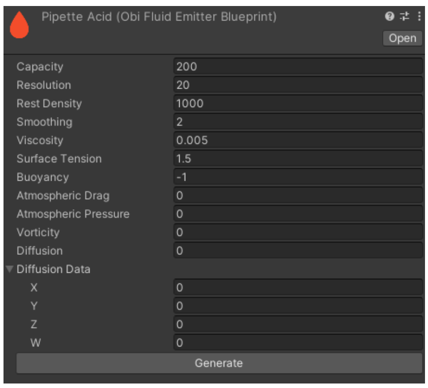

Figure 9. Properties for HCl fluid blueprint.

The liquid can be poured in the flask, on the table, or on the plate and all these objects have attached an Obi Collider so that the collision between them and the liquid gets detected. By subscribing to the *Solver_OnCollision* event it is possible to determine with which objects the liquid is colliding. On a plate, a couple of zinc granules are placed. The goal is to move them into the flask using forceps. A way to implement this would be to create a Fixed Joint between the forceps and the zinc granule, once the activate button is pressed. The zinc granule also needs to be in proximity to the forceps tip, to perform picking. On deactivation, the Fixed Joint is destroyed, and the zinc granule is released from the forceps.

Some objects that contain liquid rendered by Obi Fluid should also have the possibility to be grabbed by the user. However, since the object can be moved, it is not uncommon for liquid collisions to be missed, and for some liquid particles to fall out of the container during movement. One way to improve this, however, the liquid will still fall if the collider is moved too fast, is to set the continuous collision detection to 1, and the surface collision iterations to maximum, in the Obi Solver component.

The reaction between the HCl liquid and zinc granule forms foam. Obi Fluid allows for a very quick setup to generate foam by setting an Obi Foam Generator to the emitter of the HCl liquid. A couple of parameters need to be set, but the most important is the reference to the Particle Advector component of the foam emitter, which holds a particle system.

To emit the hydrogen bubbles in the water pot, after the tube is connected a new Obi Emitter has been created just for that. The next step is to add a bottle on top of the water pot to catch hydrogen bubbles. The bottle should therefore have 4 main states: empty state, accumulating hydrogen state, ready to burn state, and burning state.

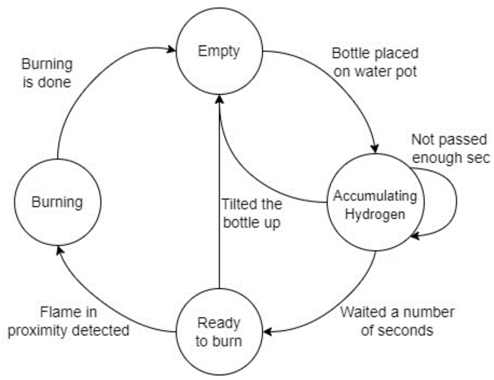

Figure 10. The state machine of the bottle object.

By utilizing a state machine (Figure 10), it is possible to dictate how the bottle should behave depending on its internal states, and which conditions should be respected to move the bottle from one state to another.

To perform burning of the hydrogen the bottle's state needs to be ready to burn. A lighter will have an Emit Flame class that will simply show the flame while the activate button is pressed. The Detect Flame Collision class will verify if the lighter tip is in the proximity of the bottle mouth, by using a trigger collider, and if the flame is also activated then burning can be performed. Figure 11 shows the result after implementing the reaction of zinc with HCl experiment.

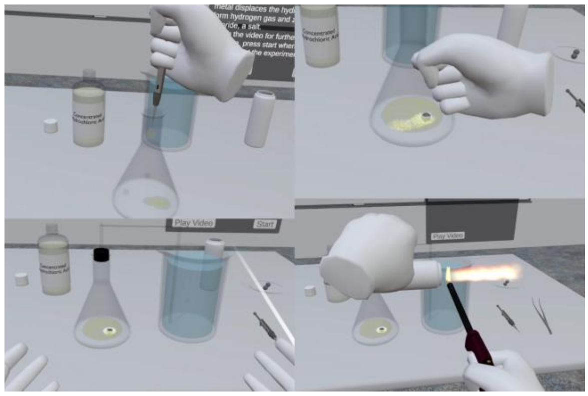

Figure 11. Reaction of zinc with HCl experiment.

Acid-base identification experiment

Liquid pouring is performed in the same way as the reaction of zinc with HCl experiment, but, additionally, this experiment also requires liquid diffusion. Two Obi Emitters are needed for liquid diffusion, one is creating the solution in the flask, and the other one is the indicator solution that is being poured by the pipette. Upon collision, the diffusion of the color should happen and for this, a diffusion channel can be used [13]. The rate of diffusion impacts how fast the diffusion will happen. In this application, channel X is used for the diffusion, the first fluid blueprint having the value 0 and the second having the value 1. On collision, the liquids will continue to change color until the value of 0.5 in channel X is reached for both fluids. The class *Obi Fluid Property Colonizer* (Figure 12), provided by the Obi plugin, maps the value from the diffusion channel to a gradient value that will determine the corresponding color of the liquid.

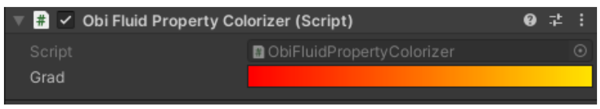

Figure 12. Obi fluid property colonizer component.

For this experiment, another method for keeping the liquid in the container while moving it can be used. The Obi Solver can also be placed inside the container, and therefore this will also move the liquid and it is not needed to rely anymore on collisions being detected or not with the container. This ensures that no matter how fast we move the container the liquid will stay inside, however, the liquid must never be poured from the container as the particles that are outside the container will still follow its movement. Figure 13 shows the simulated acid-base identification experiment and movement of a tube containing liquid.

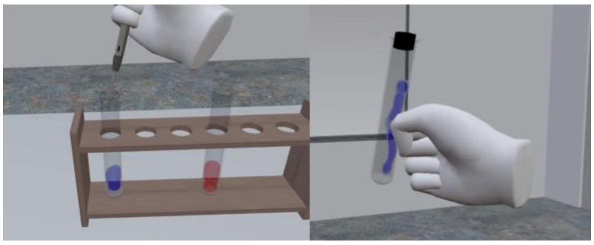

Figure 13. Acid-base identification experiment

Instructions and educational video

An instruction view is made by utilizing a unity canvas. In the instruction view, there is the possibility to view instructions by pressing the *Start* button or to view an educational video by pressing the *Play video* button. Once the video is running it can be stopped from the *Stop video* button or skipped from a skip button (see Figure 14).

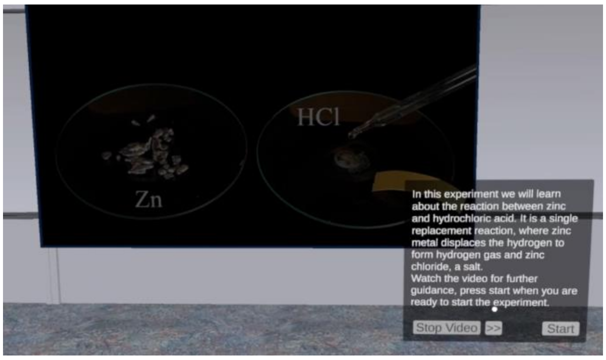

Figure 14. Instructions and educational video.

Teleportation in the scene

Teleportation in the scene is implemented by using the *Teleportation Provider* offered by the XR Interaction Toolkit. A teleportation plane is created to select where the user can teleport, and ray interactors are used to select the desired location for teleportation.

Writing on the whiteboard

To be able to write on the whiteboard texture resolutions should be changed to 2048 x 2048px. The actual writing makes use of Unity's ray cast method to detect when the marker tip is touching the whiteboard and the collision place. At the point that was last touched a small square of pixels will be drawn. Between the last point touched and the next point touched interpolation will be done to fill in the gap and give continuity to what is written [14]. How writing on the whiteboard is performed in the VemClass application is shown in Figure 15.

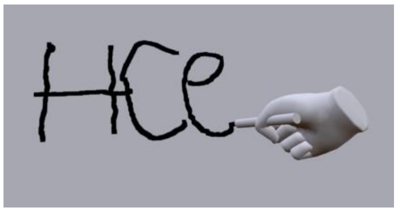

Figure 15. Writing on the table.

USER TESTING

A pilot study was conducted in which the application was tested by 7 middle school students, and by a teacher. The students' ages ranged between 13 and 14 years old. Half of them had previous experience with VR. Most of them required some additional guidance in the beginning on how to utilize the controllers to interact with the virtual objects. Some of them find it confusing which buttons to use for grabbing and activating and which object to grab. However, the users that had previous experience with virtual reality, found the controllers easy to understand. After performing this initial action, all of them were able to continue without further guidance. The users completed the experiments in a 5-to-10-minute frame. The socket interactors improved the interaction by making it possible to snap the objects into the desired places.

After utilizing the application, they were given a questionnaire, to measure the usability and learning experience for this application. They were asked to choose how much they agreed or disagreed with statements such as: I found it easy to understand how to utilize this application; I would like to use this application during chemistry lessons; I found the educational content provided in this application to be valuable; I would find chemistry lessons more engaging if VR technology was used.

Results showed that most of the students consider the application to be easy and intuitive to use, they learned quickly how to utilize it, given that some of them did not have previous experience utilizing VR. The users stated that the instructions and educational video that was provided for this application helped them to understand and perform the experiment. None of the participants stated that they experienced motion sickness. Some of them considered that they needed the instructions to be more detailed by integrating tutorials or that a voice should be added to read the instructions. Most of them strongly agree that VR would make chemistry lessons more engaging, and therefore they agree that the motivation to learn could be increased.

BENCHMARKING

The application is running steadily on a PC reaching 72fps, without frame drops, if the PC has the requirements that are specified by Meta to run Meta Quest Link. On the standalone headset, 36fps were reached as the hardware is less performant, fluid simulations are computationally expensive, and Obi Fluid requires multi-pass rendering.

CONCLUSIONS

The main contribution that the VemClass application brings is that it is an educational application that runs on a VR headset to help students in their learning process. The VemClass application has implemented a liquid simulation that utilizes Obi Fluid particle-based simulation engine, unlike other applications that are implementing a chemistry laboratory in VR. It has an intuitive interface, easy to understand and utilized by middle schoolers. The application is also highly interactive as it allows one to interact directly with the chemistry objects to perform the experiments. The level of realism in fluid simulation, especially when it comes to liquid diffusion and foam generation, was improved by utilizing the Obi Fluid engine. Possibly liquid simulation can be further improved, by utilizing ZibraAI for rendering fluids, as it utilizes AI technology that can improve the liquid rendering while also keeping a high level of performance. ZibraAI had just released Zibra Effects [15] in May 2023, and it is claimed to support VR rendering, multiple liquid types, liquid mixing, foam simulation smoke and fire, making it a viable choice for a chemistry laboratory application in VR.

As the participants that utilized this application concluded, the instructions can be further detailed, by adding tutorials to utilize this application and by providing a voice for reading the instructions. Another improvement would be to add tooltips when a hand is hovering over an object, to display the object's name, so that the user can be assured that the right object was picked. Also, information on where to place the hand to grab an object, for more complex interactions could be provided.

Overall, VemClass proves to be a valuable immersive educational application, that can provide a perspective on how VR technology can improve laboratory lessons.

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