Integrating virtual reality into active learning of molecular structures: a technologically based teaching approach

Alcides Alvear Suárez[1], Gabriel R. Flores[2], Kris Y. Gonzalez[3], Idalides J. Vergara[4], Carmen L. Carvajal[5], Yahya Masalmah[6]
[1,2,3,4,5,6]Universidad Ana G. Méndez-Gurabo, Puerto Rico
[1]aalvear@uagm.edu; [2]gflores49@email.uagm.edu; [3]kgonzalez480@email.uagm.edu; [4]ivergara@uagm.edu;
[5]carvajarc1@uagm.edu; [6]ymasalma@uagm.edu

Abstract*– We present a virtual reality application designed to improve the understanding of basic molecular structures in chemistry education. The system addresses the challenge faced by students who struggle with abstract chemical representations by enabling interactive, immersive 3D visualization. The application allows users to manipulate molecular models, access contextual information, and complete knowledge-based challenges within a virtual environment. We conducted multiple trial sessions to evaluate the system's accuracy, immersion, usability, and educational value. Feedback gathered from both students and faculty highlights the potential of VR as an effective tool for enhancing conceptual learning in chemistry.

Keywords*-- Virtual Reality, Molecular Visualization, Educational Technology, 3D Interaction, Immersive Learning, Chemistry Education.

I. Introduction

Students often have trouble visualizing concepts within the topic of molecular structures. Molecules, defined as the smallest units of a substance that retain its chemical identity, often require spatial understanding for full comprehension [20]. The main objective of this project is to facilitate the learning of the topic by using virtual reality, in which they can interact with 3D models of different molecular structures.

Using virtual reality, users can manipulate models of molecular structures in 3D in real time, observe their details and deepen their understanding of said topic. Combining reading and knowledge assessment allows for a more interactive and visual approach to help those whose learning strengths are visual by taking advantage of the unique properties of VR like immersion, real-time manipulation and spatial awareness [7].

II. Procedure

A. *Overview*

The development cycle for the project aimed to implement different features that are intuitive to the users as well as immersive. We chose to implement a Kanban model for our development cycle to maximize efficiency in short bursts of progress for a small team [4]. The process was focused on 3 primary objectives:

- Implement the core functionalities of the application within a VR environment
- Develop a database and server to manage user data, challenges, and scores.
- Consult with professionals on the topic of representing molecular structures in a scientifically accurate way during the development and implementation process.

This report shall focus on representing the progress achieved during the implementation of our virtual reality application, detailing the functionalities and integration progress.

B. *Technologies and Tools used for Development*

- Unity 6.0.0 (6000.0.36f1): Unity is the primary development platform of choice for this project in great part for its support for virtual reality applications as well as an extensive library database to assist in VR development [5].
- C# (Application Side Scripts): Easy to learn and implement, also integrated on Unity [11].
- Meta Quest 3S: This equipment is the VR headset of choice for our project. The main reason for its selection is due to its accessibility and cost efficiency [1].
- MySQL (8.3.0): A relational database management system that is used to store user information, challenge information and evaluate data of the users securely and efficiently [12].
- Node.js (v22.14.0): Runtime environment that allows you to execute JavaScript code on the server side. Manages connection between the database with the application [15].
- JavaScript (Server-Side Scripts): Programming language for communication with the database [14].

C. *Third Party Libraries Used*

- Meta XR all-in-one SDK (Oculus Integrations): Contains several Meta SDKs togethers, providing full coverage of the controls and functions for Meta Quest 3 via building blocks [18].
- 371 simple buttons packages: Includes 371 PNG buttons and 25 PNG icons. For menu aesthetics.
- Real Stars Skybox Lite: Includes 3 skyboxes.
- XR Interaction Toolkit: A high-level, component-based, interaction system for creating VR and AR experiences [19].
- XR Plugin Management: Package that provides simple management of XR plug-ins [19].

D. *Implemented Structural Diagram*

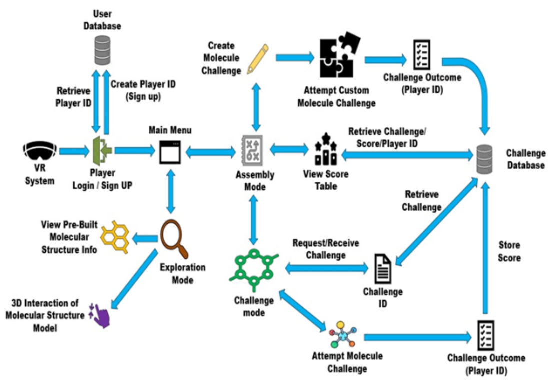

Fig. 1. Implemented Structural Diagram

To make learning more interactive in chemistry education, our project emphasizes the visualization of 3D molecular structures and the evaluation of user learning through virtual reality challenges. The key elements are described in the structural diagram, as shown in Figure 1. This diagram illustrates the flow between system interfaces, such as the database and the various game modes available to the user.

The main elements of the system include:

- VR System: The user is taken to the login menu, where they can authenticate with their credentials to access the other elements of the system. Otherwise, they can enter as guests.
- Exploration mode: In this mode, the user has access to the models of the molecules available in the system. The game mode displays the details of the molecule selected by the user, along with its 3D structural model. In addition to interacting with it such as grabbing it and inspecting it closely for a better view [13].
- Assembly Mode: This mode allows users to assemble molecules and custom challenges, which can be evaluated by other users at the leaderboard. Regarding the custom challenges:
- Users are given the elements of a molecular structure and are tasked with correctly assembling the molecule within the VR environment.
- Users can add parameters to their assembly related to molecular structures to test their knowledge on the challenge.
- Database for Users and Challenges: The database manages player ids and challenge ids, including the storage and validation of challenge information [12].
- Server for Database and Application Communication: A server is configured to manage table requests and the user sign-in and sign-up communications between the database and the VR application [15].

E. *Entity-Relationship Diagram (ERD)*

The Entity Relationship diagram was implemented as shown in Figure 2, which includes 3 tables:

- Players: Contains user credentials
- Player_scores: contains information pertaining to player scores in designated challenges.
- Challenges: Contains information on individual challenges.

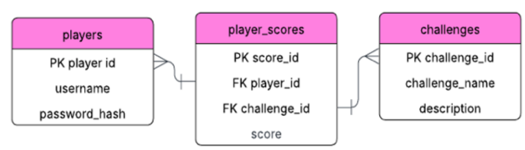

Fig. 2. ERD for database tables: players, player score, and challenges.

F. *Data-Flow Diagram*

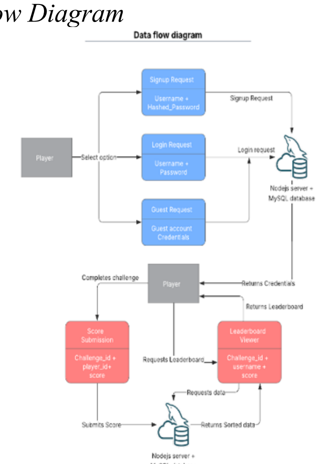

Fig. 3. Data Flow diagram of player information through the application.

The data flow of these relationships through the database within the application is shown in Figure 3. It mainly pertains to the following sequence:

- The players choose to log in, sign up or enter as guests.
- The server receives the requests and proceeds to return and create (if the user chose to sign up) the necessary credentials if authentication was successful.
- When a player submits a challenge, the submission is sent to the database to the server and stored.
- When a player chooses to see the leaderboard of a particular challenge, the application requests the server the necessary score, challenge and players and sorts the leaderboard into the top 5 scores.

G. *Front-end Implementation*

The objectives proposed in the kanban model for the front-end implementation were focused on the game logic, such as the implementation of menus, interaction of molecules, and creation of challenges. The project has implemented two game modes: exploration mode and assembly mode, with the latter implementing a custom challenge mode to add challenge parameters.

The implementation of the virtual interface for the user focuses on being simple and user-friendly. The following interfaces were created for the application.

a. Main menu

1. Login Menu Layout: The interface aims to authenticate the user to the system, as shown in Figure 4. It can also authenticate as a guest to enter the app without using username and password.

Fig. 4. Login Menu

b. Assembly game mode

1. Molecule Selector Menu: The user is given a virtual environment where it can select the molecule of their choice to assemble. The selector is shown in Figure 5.
2. Assembly game logic: By using snap interaction, a script is used to verify if the snap interactor (the atom or bond component) has an interactable (place for attachment). When every interactor has an interactable, if all interactors have their correct tag, it will display a completion panel depending on if the molecule is correctly or incorrectly assembled.
3. Timer Panel: When the molecule is selected, the timer is immediately started. When the molecule is assembled, the timer is stopped and the time spent in the assembly is recorded in the database and towards the leader board. The example of the timer is shown in Figure 6.
4.

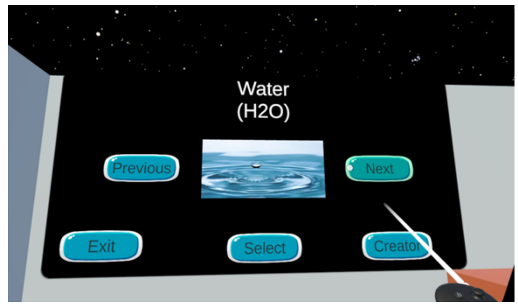

Fig. 5. Molecule selector panel

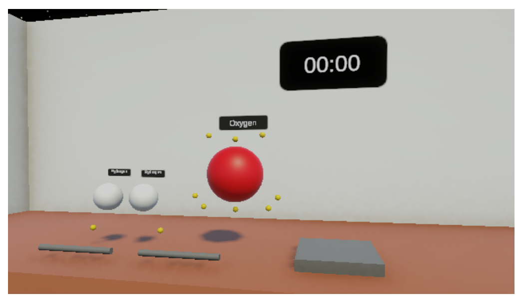

Fig. 6. H2O molecule components for its assembly with the timer.

5. Leaderboard: The user can see other players score during the virtual experience. Once they complete the assembly, the time spent is uploaded along its player id as score. An example of the leaderboard is shown at Figure 7.

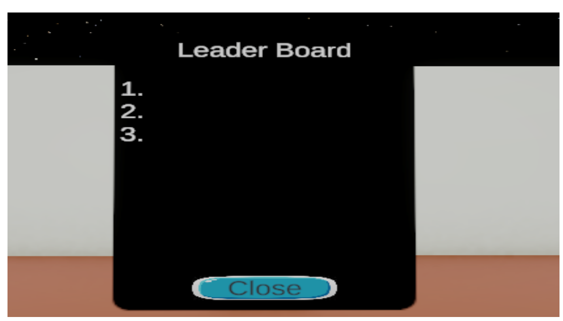

Fig. 7. Leaderboard panel example.

c. Custom creator challenge mode

1. Challenge parameters creator: The user can add parameters for its assembly, like assemble the molecule by verifying its electron count. The parameter selector is shown in Figure 8. This prototype only uses the H2O model in the creator mode.

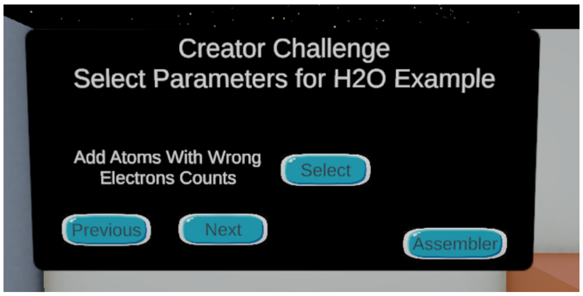

Fig. 8. Creator challenge selector for the H2O molecule example.

d. Exploration game mode

1. Molecule information panel: Using the molecule selector, it displays the molecule completely assembled and its information panel with its respective description. The example of the molecule description at the exploration mode is shown in Figure 9.
2. Molecule interaction: The user can interact with the molecule itself by grabbing it.

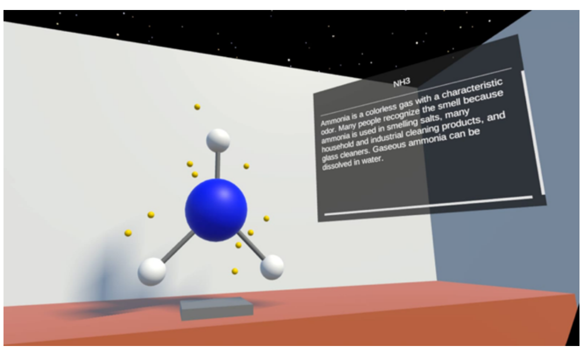

Fig. 9. The 3D model of the NH3 molecule with its information panel with its description.

H. *Back-end Implementation*

The objectives proposed in the kanban model for the back-end implementation focus on enabling communication between the Unity client, Node.js server, and a MySQL database [4], [12], [15]. The project has implemented sign-in and sign-up features, as well as leaderboard for players that completed an assembly using a challenge id to see their score.

a. MySQL

The database relates the players' IDs with the IDs of the molecular structure challenges they have attempted, and the time elapsed in the challenge to complete their score.

b. Node.js

Handles Communication between the MySQL database and the application by using UDP (User Datagram Protocol) to allow the server to broadcast its port number.

c. Unity Client Side

Makes requests to the Node.js server with UDP in order to implement the sign-in and sign-up functions.

Upon completing a molecular structure challenge, the application sends the player's score to the server for storage in the database.

The application requests the leaderboard data by sending the relevant challenge id and player id to the server. The backend responds with a sorted list of scores, allowing the client to display the top-performing players.

III. Requirements

A. *Functional Requirements*

a. User Access and Authentication

1. Account creation tools for sign-up and log-in.
2. Assign each user their own User ID.
3. Login interface.
4. User authentication.
5. Guest authentication.
6. Offline entry.

b. Core Features: Molecule Visualization and Interaction

7. Capability to navigate the user interface with VR control systems.
8. Implement a navigation menu for assembly game mode.
9. Implement a navigation menu for the creator mode inside the assembly game mode.
10. Implement a navigation menu for exploration game mode.
11. Capability to view, grab and interact with a 3D model of a molecular structure.
12. Display if the user has assembled the molecule correctly or incorrectly.
13. Provide an info panel that details the type of molecule and its information.
14. Allow users to interact individually with each molecule.
15. Allow users to set challenge parameters to test their assembly skills.

16. Include a selection of different molecules (CO_2, H_2O, NH3, H_2SO_4)

c. Challenge Creation and Engagement

17. Mode to add parameters and create challenges based on existing molecular structures.
18. Allow users to view a scoreboard of attempted challenges and custom challenges.
19. Allow users to view the score of other players who attempted a challenge parameter.
20. Provide an interface with easy-to-follow instructions for challenge customization.
21. Include hints for challenges.

d. Database and Server Integration

22. Implement a MySQL database to store player account information and scores.
23. Establish a Nodejs server to serve as a bridge between our VR Unity application and the database.
24. Handle user authentication requests via WebSocket communication.
25. Use UDP broadcasting to allow Unity to automatically discover the server on a network.
26. Ensure that the backend communication is efficient.

e. Data Storage and Real-Time Functionality

27. Storage for challenge exercises tested by the user.
28. Storage for user information.
29. Storage for the player's challenge results evaluation with their user ID.
30. Allow real-time updates.

f. Security

31. Secure data access using hashing for user data protection.
32. Security for user information and challenge information.

B. Non-Functional Requirements

a. Performance

33. Low latency.
34. Smooth experience.
35. Responsive controls.
36. Ensure frame rate stability.
37. Allow compatibility with minimal performance requirements of Meta Quest 3.

b. Scalability

38. Allow support for additional content.

c. Ease of Maintenance

39. Adhere to Unity C# best practices.
40. Proper code documentation.
41. README files for guidelines.

d. Usability

42. Include tutorials to help new users with controls and features.
43. Have responsive and easy to use controls for an easy learning curve.

IV. Results

The application underwent two public trial runs. The first took place on April 24, 2025, during the EXPLORATEC event hosted at the “Centro Criollo de Ciencia y Tecnología del Caribe (C3Tec)”. This initial demonstration focused on evaluating the core functionalities of the application, including the basic login and sign-up system, interactive manipulation of three molecular structures, and the performance of both the exploration and assembly modes. Groups of visiting students attended the application, and their feedback highlighted several areas for improvement. Most notably, users expressed the need for better depth perception to gauge molecule placement accurately, increased ease of access in the user interface, and clearer feedback mechanisms during the assembly of molecular structures.

In response to this feedback, we implemented multiple improvements in preparation for the second public demonstration, which took place during the Engineering Day event at the Ana G. Méndez University, Gurabo Campus, on May 19, 2025. By this stage, the application had full integration with database and server functionalities, including guest access, user login and logout features, and a system for tracking and displaying scores per challenge via a leaderboard. Front-end enhancements were also made, such as clearly labeled electron counts on atomic models, improved level design to aid spatial clarity and depth discernment, and visual socket indicators to guide users in placing atoms correctly during assembly. Additionally, an early prototype of a Custom Challenge Mode was introduced, which tasked users with identifying and assembling correct molecular structures using atoms differentiated by electron count.

The second round of feedback provided us with valuable insights into future development. Users expressed interest in having the application visually indicate when electrons are correctly assembled, as well as incorporating a wider variety of bond types, including metallic and ionic bonds. Suggestions were also made regarding further refinement of the user interface to enhance overall usability and immersion.

V. Conclusions

The tests conducted demonstrated that the use of virtual reality equipment provided users with an immersive and interactive experience, which significantly contributed to the improvement of knowledge retention. The project was consolidated as a valuable complementary educational tool for the teaching of chemistry.

Furthermore, the implementation and demonstration in two public trials confirmed both the technical and pedagogical feasibility of the application, highlighting its potential to facilitate the learning of more complex molecular concepts in future scenarios.

Finally, the results obtained support the need to continue expanding the molecular structure database by incorporating more advanced models and functionalities. Similarly, further optimization of usability and visual interface design is projected, with the aim of maximizing both the didactic effectiveness and the user experience.

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