ChemistryVR: Simulating Chemistry Experiments in Virtual Laboratories

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Figure 1: 3D virtual chemistry laboratories. (a) The room layout of the virtual laboratory. (b) Some experimental apparatus. (c) Virtual manuals showing experimental operations.

ABSTRACT

Experiment is an essential part of chemistry education. However, it is equipment- and space-demanding, and sometimes risky. Immersive and interactive simulations in Virtual Reality (VR) can address these issues. In this project, we developed a virtual laboratory based on China's ninth grade chemistry textbook published by People's Education Press. The system provides safety training and step-bystep tutorials so that students can learn from interactive simulations and observations of realistic experimental phenomena in a safe condition. Our system provides a risk-free approach and effectively supports practice-led and experiential learning of chemistry.

Keywords: virtual reality, simulation, chemistry education

1 INTRODUCTION

Chemistry is an experimental science that requires students to learn by doing through experiments with laboratory apparatus and chemicals. However, conducting real chemistry experiments is risky for students who lack basic knowledge and safety training for laboratory work. Additionally, chemistry education presents challenges in terms of the costs in space, laboratory facilities, chemical management, and monitoring of students in the event of safety concerns. Conducting chemical experiments can be risky, expensive, and labor-intensive. In this project, we designed and developed a virtual laboratory that allows students to learn chemistry experiments through simulations in Virtual Reality (VR). After receiving safety training, students can move around in the virtual laboratory to explore the common-seen laboratory apparatus and chemicals, follow detailed instructions to practice chemistry experiments, and observe real-time experiment phenomena in detail. Our system realized the following functions that are essential for chemistry education: (1) safety training, (2) active experimentation with laboratory apparatus and chemicals, and (3) real-time simulations of chemistry experiments. The system supports practice-led learning of chemistry and can be widely applied in middle and high school chemistry education in China.

2 BACKGROUND

Virtual Reality (VR) has features of immersion, interaction, imagination, and involvement, and has shown great potentials in education by making learning more motivating and engaging. For chemistry education specifically, lab safety [1] remains to be a major concern

that need to be addressed regardless of the teaching medium. In addition, active experimentation is significant for chemistry education, and is richly afforded by virtual laboratories. A recent work [2] has reviewed existing 2D and 3D virtual chemistry laboratories and identified the following issues actual virtual experiments: (1) lack of realism and immersion in 2D environments, (2) lack of control over experiments (video only), (3) unrealistic control of 3D objects through menus and control boxes, (4) no simulation of chemical reactions, and (5) only English language is supported. Based on these findings, our work aims to develop a 3D virtual chemistry laboratory that (1) presents an realistic and immersive environment, (2) supports interactions with various forms of media, include videos, texts, and 3D objects, (3) presents direct manipulation of 3D chemical apparatus to simulate realistic chemistry experiments, (4) demonstrates real-time simulation effects of chemical reactions, and (5) provides instructions in Mandarin Chinese.

3 DESIGN AND IMPLEMENTATION

The design and implementation of our virtual chemistry laboratory strictly followed the China's ninth grade chemistry textbook [3]. In this section, we present the implemented functions in detail.

3.1 Apparatus

Our VR laboratory was built using a computer with Intel Core i7-12700H CPU @ 3.60GHz, 32GB RAM, NVIDIA GeForce RTX 3080 graphics card with 10GB RAM, and deployed on an Oculus Quest 2. The systems were built using Unity (version 2021.3.6) and two packages: VR Interaction Framework¹ and Liquid Volume Pro 2^2 . We used 3D Studio Max 2016 and Rhino 7.0 to build the 3D models and set up virtual scenes. The demo videos were edited using Adobe Premiere.

3.2 Chemistry Lab Environment

We simulate a realistic chemistry laboratory environment by setting up experimental tables, chairs, cabinets, and common-seen apparatus (see Figure 1). Specifically, 3D models of beakers, test tubes, measuring cylinders, microscopes, wire shelves, funnels and other chemical apparatus are presented on the experimental tables. In addition, chemicals are also displayed in the corresponding apparatus to achieve better simulation results.

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¹https://assetstore.unity.com/packages/templates/ systems/vr-interaction-framework-161066

²https://assetstore.unity.com/packages/vfx/shaders/ liquid-volume-pro-2-129967

3.3 User Interface Design

The system provides safety training, experiment instructions, quizzes, and system controls through user interface design (see Figure 2). First, a video is presented at the start of the virtual laboratory experience to explain safety regulations and to help users understand the importance of safety in a chemistry laboratory. Second, chemical laboratory specification documents and operating instructions are provided to help users get familiar with laboratory safety concerns and operating specifications. Third, an interactive quiz with multiplechoice questions is set up to check users' understanding of safety issues. Fourth, navigation menus with virtual buttons allow users to choose different experiments.



Figure 2: User interfaces for users to view (a) tutorial videos, (b) instructions, (c) complete quizzes, and (d) switch between experiments.

3.4 Interaction Design

The virtual laboratory supports 3D interactions and direct manipulations (see Figure 3). Interactable objects are indicated by prompt rings. By pressing the grip button on the controller, users can manipulate the lab apparatus; by pressing the trigger button, users can achieve teleport locomotion. Ray-based selection was implemented for user interface interactions and system control. For some experimental interactions, such as manipulating the dropper to drop liquid chemicals, users can complete the operations by following the instructions presented around the operation desks.

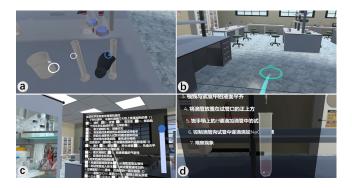


Figure 3: Interaction design. Users can (a) grab an experiment apparatus, (b) move around using teleport, (c) interact with the UIs using raycasting selection, and (d) conduct an experiment using controllers.

3.5 Chemistry Experiment Simulations

To simulate realistic experimental phenomena, we realized the effect of liquid color using Unity Shaders and the change of effects is triggered through collision detection. Figure 4 shows a demonstration of an acid-base titration experiment. When dropping sodium hydroxide solution (NaOH) into the phenolphthalein solution, the phenolphthalein will turn red in the presence of alkali. Students can observe the phenomena that the solution changes from colorless to red gradually in real time. Step-by-step instructions are provided to students to show the correct experiment operations.

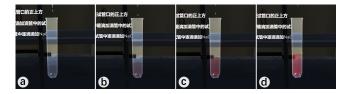


Figure 4: An acid-base titration experiment: (a) phenolphthalein solution in the test tube, (b-d) adding sodium hydroxide solution using the dropper, the color gradually changed from colorless to red.

4 DISCUSSION

Our virtual laboratory design aligns with the Chinese nine-year compulsory education syllabus and provides essential assistive teaching tools, including safety training, standardized lab instructions, and step-by-step tutorials for experiments. The system has three main advantages. First, it effectively addresses safety-critical issues in chemistry education throughout the virtual laboratory experience. Second, it supports experiential learning through active experimentation. By following detailed experimental steps and observing the phenomena, students can better understand the theoretical knowledge. Third, simulating chemical experiments in VR can significantly reduce the cost in facilities and spaces. This system can be used for online and distant learning. For future work, we plan to strengthen the safety feature by providing warnings to students upon dangerous operations in time. In addition, we plan to include task-oriented games, such as finding the required chemicals for an experiment based on the appearance characteristics, to engage students in exploratory and game-based learning.

5 CONCLUSION

In this project, we built a virtual laboratory for middle school chemistry education to help students conduct experiments in a safe environment. We simulated a realistic virtual laboratory environment populated with various chemistry apparatus and reagent, designed user interfaces and 3D interactions for safety training and active experimentation, and created simulations of chemistry experiments with real-time phenomenon changes based on user interactions with the laboratory apparatus and chemicals. The system provides a onestop solution for middle school chemistry education, from learning safety operations in chemistry laboratories to conducting experiments learned from the textbooks. Our system demonstrates the potentials of VR technology use in chemistry education, providing a risk-free, highly interactive, and cost-effective solution to the teaching and learning of safety-critical subjects.

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