ChemistryVR: Enhancing Educational Experiences through Virtual Chemistry Lab Simulations

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Figure 1: Overview of the 3D virtual chemistry laboratory. (a) Spatial layout of the virtual laboratory environment. (b) Selection of virtual experimental apparatus. (c) Interactive virtual manuals demonstrating experimental procedures.

Abstract

Experiments are an essential component of chemistry education. However, they often demand significant equipment and space and can sometimes pose safety risks. Immersive and interactive simulations in Virtual Reality (VR) offer a solution to these challenges. Therefore, we developed a virtual laboratory based on the ninthgrade chemistry textbook published by the People's Education Press in China. The system includes safety training and step-by-step tutorials, enabling students to learn through interactive simulations and observations of realistic experimental phenomena in a safe environment. Hands-on practice of chemistry experiments in VR helps prevent dangerous and unexpected outcomes caused by experimental errors. Our system provides a risk-free approach that effectively

supports practice-led and experiential learning in chemistry. Additionally, our system integrates theoretical knowledge with practical applications, aligning meticulously with the official textbook. This comprehensive approach enables students to seamlessly transition from theory to practice, enhancing their understanding of chemistry concepts. Consequently, students are better prepared for both standardized assessments and real-world laboratory experiences.

CCS Concepts

 Computing methodologies → Computer graphics; Virtual reality; • Applied computing → Interactive learning environments; • General and reference → Experimentation.

Keywords

Virtual laboratory, Hands-on, Experimental simulation, Chemistry education

ACM Reference Format:

Guanxuan Jiang, Xuansheng Xia, Yue Li, Hai-Ning Liang, and Pan Hui. 2024. ChemistryVR: Enhancing Educational Experiences through Virtual Chemistry Lab Simulations. In SIGGRAPH Asia 2024 Educator's Forum (SA Educator's Forum '24), December 03–06, 2024, Tokyo, Japan. ACM, New York, NY, USA, 5 pages. https://doi.org/10.1145/3680533.3697068

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SA Educator's Forum '24, December 03–06, 2024, Tokyo, Japan

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ACM ISBN 979-8-4007-1136-7/24/12

https://doi.org/10.1145/3680533.3697068

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1 Introduction

Chemistry, as an experimental science, requires hands-on learning through practical experiments utilizing laboratory apparatus and chemicals. However, conducting real chemistry experiments poses significant risks for students lacking fundamental knowledge and safety training in laboratory procedures. Moreover, chemistry education presents challenges in terms of spatial requirements, laboratory facilities, chemical management, and student supervision to address safety concerns [Bai et al. 2022; Schenk et al. 2018]. The intrinsic hazards, financial constraints, and resource-intensive characteristics of chemical experimentation increasingly impede student engagement in laboratory work within conventional educational frameworks, particularly in the context of China's educational landscape [Qing et al. 2010]. The proliferation of virtual chemistry laboratories utilizing virtual reality (VR) technology has gained considerable momentum in recent years [Sreekanth et al. 2022; Tatli and Ayas 2013]. These innovative platforms are proving increasingly valuable in educational contexts, primarily due to their inherent advantages of portability, cost-effectiveness, and elimination of physical safety risks associated with traditional laboratory environments. Nevertheless, existing virtual chemistry laboratories predominantly focus on experimental procedures, often neglecting comprehensive safety guidelines and realistic experimental outcomes [Han et al. 2017].

Within the context of China's educational framework, facilitating universal student participation in hands-on chemistry experiments poses considerable challenges. The fundamental objective of chemistry experimentation is to empirically validate theoretical principles; however, the practical realization of such experiments is frequently impeded by a multitude of constraints in real-world educational settings [Wang et al. 2018]. Although students are routinely assessed on their comprehension of safety procedures and experimental observations during examinations, a significant proportion lack authentic laboratory exposure [Hou et al. 2023; Huang 2020]. This deficiency in firsthand experimental engagement represents a notable shortcoming in their scientific training, potentially impacting their deeper understanding of chemical processes and experimental methodologies.

In this project, we have designed and developed a virtual laboratory system that enables students to engage in chemistry experiments through immersive simulations in VR. After completing comprehensive safety training, students can navigate the virtual laboratory environment, examine common laboratory apparatus and chemical substances, follow step-by-step instructions to conduct chemistry experiments and observe detailed, real-time experimental phenomena. Our system implements three essential functions crucial for chemistry education: (1) comprehensive safety training, (2) interactive experimentation with laboratory apparatus and chemicals, and (3) real-time simulations of chemical reactions and processes. To reinforce safety protocols, the system provides videos detailing chemical laboratory safety specifications and interactive safety questionnaires, ensuring students fully grasp experimental requirements and operational protocols. A central focus of the project is the high-fidelity simulation of chemical experiments in VR, employing Unity's shader component to accurately simulate liquid behaviour and appearance. This system facilitates practice-led

learning in chemistry and has the potential for widespread application in secondary and high school chemistry education throughout China.

2 Background

Over the past two decades, the rapid advancement of Virtual Reality (VR) technology has facilitated its application across diverse fields. In education, VR has demonstrated significant potential by enhancing student motivation and engagement in the learning process. Specifically in chemistry education, laboratory safety remains a paramount concern that must be addressed regardless of the instructional medium [Ménard and Trant 2020]. Moreover, active experimentation, which is crucial for chemistry education, is abundantly afforded by virtual laboratories. Recently, Ali and Ullah [Ali and Ullah 2020] reviewed existing 2D and 3D virtual chemistry laboratories and identified several issues in current virtual experiments: (1) insufficient realism and immersion in 2D environments, (2) limited control over experiments, often restricted to video demonstrations, (3) unrealistic manipulation of 3D objects through menu-based interfaces and control boxes, and (4) absence of chemical reaction simulations. These findings are crucial for the iterative development of the virtual chemistry lab, as they provide a clear understanding of the features that require enhancement.

2.1 VR-Assisted Chemistry Teaching

A need analysis has shown that chemistry teachers hold a positive attitude towards the use of VR chemistry laboratory for teaching chemistry experiments [Solikhin et al. 2019]. Specifically, it is beneficial to use VR for safety training and to provide a risk-free approach for active experimentation with the chemicals.

Providing an immersive experience that makes students feel as though they are physically present in a chemistry laboratory is crucial. This heightened sense of immersion encourages students to pay closer attention to each step of their operations [Reeves et al. 2021]. Rather than merely observing others conduct experiments, students interact directly with the chemical apparatus to complete experiments themselves. This approach poses significant challenges for interaction design, as actions like clicking and dragging differ from real-world operations [Hofstein et al. 2013]. This aspect has been either overlooked or inadequately addressed in previous virtual chemistry laboratories. This is particularly significant for students in mainland China, as such topics are often included in their entrance examinations. Thus, refining each gesture and accurately simulating the positioning and operations of experimental equipment is crucial for providing an immersive and realistic chemistry lab experience.

Incorporating VR as an adjunct in the chemistry curriculum is crucial, particularly for students whose behavioural skills are not yet fully developed [Kong et al. 2022]. Meanwhile, providing safety operation guidelines within a virtual chemistry laboratory is essential; however, this aspect is often neglected [Chan et al. 2021]. Our system aims to bridge this gap, enabling students to perform experiments safely and independently within our platform. Our system focuses on chemistry-required experiments in middle and high school textbooks, highlighting potential safety issues that may arise during these experiments. This approach allows students

to learn effectively in a virtual environment and only proceed to hands-on experiments after successfully passing the assessments.

2.2 Mainland China Chemistry Education

In the context of middle and high school education in China, the vast majority of assessments are conducted through written examinations [Yu et al. 2018], and the subject of chemistry is no exception [Yin and Buck 2015]. The chemistry components of both the high school entrance examination and the college entrance examination, also known as Gaokao [Pires and Duarte 2019]. These examinations encompass the assessment of students' understanding of chemical phenomena, experimental procedures, and safety knowledge related to chemical experiments. Although these assessments are administered in the form of written tests, they nonetheless serve as an alternative method to gauge students' comprehension of chemical experiments. As a result, many students have limited opportunities to engage directly with a chemistry laboratory. This limitation is primarily due to concerns regarding safety and cost, as well as the perception that rote memorization is a more time-efficient method of learning. However, such an approach lacks the intuitive and hands-on experience that is essential for a comprehensive understanding of chemistry. The discipline of chemistry inherently requires active experimentation and practical engagement to fully grasp its principles and applications.

Based on these considerations and situations, our work aims to develop a 3D virtual chemistry laboratory simulation system that enables Chinese students to learn required safety chemistry laboratory protocols and conduct experiments as they would in a real-world setting, especially for mainland Chinese students. Additionally, we expect to enhance students' retention of chemical experiment phenomena and their understanding of safety protocols through learning within this system, ultimately improving their performance in examinations. Therefore, the system should (1) present a realistic and immersive environment where students can observe, navigate, and learn safety protocols; (2) support interactions with various forms of media, including videos, texts, and 3D objects; (3) enable direct manipulation of 3D chemical apparatus to simulate realistic chemistry experiments; and (4) demonstrate real-time simulation effects of chemical reactions in detail, fully consistent with the content covered in the textbook.

3 Design and Implementation

The design and implementation of our virtual chemistry laboratory strictly followed China's ninth-grade chemistry textbook [People's Education Press 2019]. In this section, we present the implemented functions in detail.

To achieve a high degree of experimental authenticity, we have meticulously focused on the apparatus utilized, the virtual environment, the interface design, the interaction design, and the simulations of chemistry experiments. In our virtual laboratory, we simulate the instruments, experimental phenomena, and operation steps of real chemical experiments. This approach aspires to provide an effective auxiliary tool for teachers and students in middle schools, potentially replacing certain functions of a traditional laboratory. This allows students to complete experiments within a safer environment.

The project ultimately implements several key functions: students can move freely within the laboratory, select an experimental table to initiate an experiment, and choose specific experiments from a pop-up menu. They can grasp the equipment on the experimental table to perform various experimental operations, with visual highlights confirming actions such as pouring or dispensing experimental liquids. Various liquid properties, including density and color, are configured using a physics engine to accurately simulate the flow effects of different liquids, color changes upon mixing, precipitation, and other chemical phenomena.

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 a Meta Quest 2. The systems were built using Unity (version 2021.3.6) and two packages: VR Interaction Framework 1 and Liquid Volume Pro 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 Laboratory Environment

We have meticulously emulated the laboratory environment based on illustrative examples from the official textbook. A white screen has been centrally configured in the virtual environment to present chemical safety videos. The virtual chemistry laboratory includes experimental tables, chairs, cabinets, and common apparatus (see Figure 1) to enhance the authenticity of the simulation. Specifically, 3D models of beakers, test tubes, measuring cylinders, microscopes, wire shelves, funnels, and other chemical apparatus are presented on the experimental tables. Additionally, chemicals are displayed in the corresponding apparatus to enhance the simulation's realism. Importantly, these pieces of equipment are not merely static images; they are interactive and can be picked up and examined by the user.

3.3 Safety Training, Instructions, and Quiz System

The system offers safety training, experiment instructions, quizzes, and system controls through a user interface design (see Figure 2). Firstly, a video is presented at the onset of the virtual laboratory experience to explain safety regulations and to emphasize the importance of safety in a chemistry laboratory. Secondly, chemical laboratory specification documents and operating instructions are provided to acquaint users with laboratory safety concerns and operating procedures. Thirdly, an interactive quiz with multiple-choice questions is implemented to assess users' understanding of safety issues. Lastly, navigation menus with virtual buttons enable users to select different experiments.

3.4 Interaction Design for Experiments

The virtual laboratory supports 3D interactions and direct manipulations, as illustrated in Figure 3. Interactable objects are highlighted by prompt rings. Users can manipulate laboratory apparatus by

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

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



Figure 2: User interfaces depicting various aspects of the virtual laboratory system: (a) tutorial videos for safety training, (b) detailed laboratory instructions, (c) an interactive quiz system for assessing user understanding, and (d) experiment control menus for selecting and navigating different experiments.

pressing the grip button on the controller, and achieve teleport locomotion by pressing the trigger button. When holding a chemical apparatus, rotating and moving the controller will result in corresponding changes to the apparatus in the interface. For operations such as pouring, we utilize highlight rings to achieve alignment functionality. Ray-based selection is employed for user interface interactions and system control. For specific experimental tasks, such as using a dropper to dispense liquid chemicals, users can complete the operations by following the instructions displayed around the operation desks.

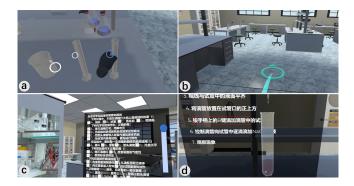


Figure 3: Interaction design: (a) users can grab experimental apparatus, (b) navigate the environment using teleportation, (c) interact with user interfaces through raycasting selection, and (d) conduct experiments using controllers.

3.5 Chemistry Experiment Simulations

To simulate realistic experimental phenomena, we employed Unity Shaders to render the effect of liquid color changes, with these changes being triggered through collision detection. Figure 4 illustrates an acid-base titration experiment. When sodium hydroxide solution (NaOH) is added to a phenolphthalein solution, the phenolphthalein turns red in the presence of an alkali. An empty object

with a 'Collider' represents the upper surface of the liquid chemicals. Students can observe the real-time, gradual transition of the solution from colorless to red, indicating a linear process rather than an instantaneous change. Additionally, the shader level of the experimental apparatus increases due to the rising level of the liquid mixture. Step-by-step instructions are provided to guide students through the correct experimental procedures. These instructions are displayed in the background, enabling students to refer to the guidance while actively conducting experiments. This approach enhances learning efficiency, accuracy, and adherence to experimental protocols.

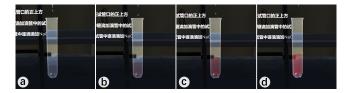


Figure 4: An acid-base titration experiment can be described as follows: (a) A phenolphthalein solution is placed in the test tube. (b-d) Sodium hydroxide solution is then added dropwise using a dropper, resulting in a gradual color change from colorless to red.

4 Discussion

Our virtual laboratory design is strictly aligned with the Chinese nine-year compulsory education syllabus, with essential assistive teaching tools, including safety training, standardized lab instructions, and step-by-step tutorials for experiments. The system offers three primary advantages compared to previous relevant applications. First, it effectively addresses safety-critical issues in chemistry education throughout the virtual laboratory experience. Second, it supports experiential learning through active experimentation, mirroring the operation gestures and experimental procedures used in real-world experiments. By following detailed experimental steps and observing the resulting phenomena, students can gain a deeper understanding of theoretical knowledge. The design of chemical experiment phenomena strictly adheres to the descriptions in the textbooks, thereby deepening students' understanding of theoretical knowledge and aiding them in achieving better performance in theoretical examinations. Third, simulating chemical experiments in VR can significantly reduce costs associated with laboratory facilities and physical space. Additionally, this system can be utilized for online and distance learning.

The subsequent iterations will increase both the variety and quantity of chemical experiments beyond the original scope to encompass a broader range of chemistry courses. By incorporating random experiments, the project aims to provide students with a wider array of experimental equipment and chemicals, enabling them to freely explore the reaction phenomena between different chemical substances. However, this expansion poses significant challenges for developers and requires extensive testing over a prolonged period. We plan to enhance the safety features by providing timely warnings to students when hazardous operations are detected. Additionally, we intend to incorporate task-oriented games,

such as identifying required chemicals based on their appearance characteristics, to engage students in exploratory and game-based learning. The system will also evaluate students' performance at the conclusion of each experiment. Due to the high cost of VR devices, not all schools can afford to equip multiple VR systems. Therefore, to facilitate integration into real-world chemistry education, the project will be adapted for both VR and PC platforms. This adaptation will enable users on different devices to conduct experiments and perform other interactive operations within the same virtual laboratory via the Internet.

5 Conclusion

In this project, we developed a virtual laboratory aimed at enhancing middle school and high school chemistry education by enabling students to conduct experiments in a safe and controlled environment. We created a highly realistic virtual laboratory environment, complete with various chemistry apparatus and reagents. Our design included user interfaces and 3D interactions for safety training and active experimentation, along with simulations of chemistry experiments that exhibit real-time phenomena based on user interactions with laboratory apparatus and chemicals. The system serves as a comprehensive solution for mainland Chinese middle and high school chemistry education, encompassing everything from learning safety operations in chemistry laboratories to performing textbook experiments. Our system illustrates the potential of VR technology in chemistry education, offering a risk-free, highly interactive, and cost-effective approach to teaching and learning safety-critical subjects. By effectively replicating a real chemistry laboratory in a virtual setting, we have increased student engagement and alleviated teaching pressure on educators.

Compared to previous research on chemistry education and existing VR chemistry simulation applications, our approach is specifically tailored to the contextual needs and educational framework of students in mainland China. Looking forward, we plan to expand the variety of experiments available and involve experienced chemistry teachers in refining the safety tips and precautions sections. Future iterations will be informed by feedback from students and teachers to ensure continuous improvement. This initiative is of significant importance to students, as it allows them to conduct experiments independently in a safe environment, rather than merely learning and observing experimental phenomena through recorded videos.

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