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Chemisim: A Web-based VR Simulator for Chemistry Experiments

Hoang-Minh Le*
University of Science
Vietnam National University
Ho Chi Minh City

Gia-Huy Nguyen†
University of Science
Vietnam National University
Ho Chi Minh City

Viet-Tham Huynh‡
University of Science
Vietnam National University
Ho Chi Minh City

Minh-Kha Le§
Faculty of Chemistry
University of Science
Vietnam National University
Ho Chi Minh City

Minh-Triet Tran¶
University of Science
John von Neumann Institute
Vietnam National University
Ho Chi Minh City

Tam V. Nguyen‖
Dept. of Computer Science
University of Dayton

Thanh Ngoc-Dat Tran**
University of Science
Vietnam National University
Ho Chi Minh City

Figure 1: A chemistry experiment using our proposed Chemisim system.

Abstract

In developing countries, high schoolers rarely have opportunities to conduct chemical experiments due to the lack of facilities. Therefore, chemistry experiment simulation is an alternative environment for students to do the chemistry lab assignments. Despite the need of creating virtual simulations to expand the application usability, it is challenging to synthesize a realistic environment given the limited computing resources. In this paper, we propose Chemisim, a highly realistic web-based VR laboratory simulation for students with high quality and usability. In particular, we make use of the fluid simulation system to mimic real chemical reactions. The implemented simulation was based on the chemistry assignments in the national education system, consulted by chemical teachers. Then we deployed the simulator on the web to promote a wide range of students usage. The system was evaluated by collecting and analyzing feedback from chemical teachers based on four criteria, namely, convenience, realism, functionality, and preferences. Our experimental findings address educational challenges and produce innovative technical solutions to solve them in developing countries.

*e-mail: lhminh18@apcs.fitus.edu.vn
†e-mail: nghuy18@apcs.fitus.edu.vn
‡e-mail: hvtham@selab.hcmus.edu.vn
§e-mail: lmkha@hcmus.edu.vn
¶e-mail: tmtriet@fit.hcmus.edu.vn
‖e-mail: tamnguyen@udayton.edu
**e-mail: tndthanh@selab.hcmus.edu.vn (corresponding author)

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Index Terms: Human-centered computing—Visualization—Visualization techniques; Human-centered computing—Visualization—Visualization design and evaluation methods

1 Introduction

There are experiments conducted highlighting the chemical simulation's effectiveness for student development [1–3, 21]. It proves the vital role of simulation in the educational aspect, particularly in chemistry [5] [6]. In developing countries, most high school students encounter a lack of experimental facilities. In chemistry class, students rarely have a chance to use a physical laboratory to conduct experiments [7]. Therefore, online simulations play a major role in education not only because of the realistic models and reactions they provided but also because students can constitute safe environments in which they can repeat processes without any risk to perceive easier concepts and theories [8]. A well-developed simulated system can provide an accessible environment for students studying, also boosting the studying experience in secondary schools. Producing a high graphical laboratory based on national lessons deploying on an easy-to-reach platform is an effective solution for education development.

Currently, there are many related works to solve the problem of experimental simulation in many fields. The approach using virtual reality technology can be mentioned as one of the most popular ones. We can find their solution at [9–13]. Additionally, Labster's Virtual Lab Simulation is a more prominent and comprehensive approach [14]. On the public site of [14], we can easily find demo videos of some specific experiments. On the other hand, augmented reality applications are also being researched and put into applications

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to serve mobile phone users. Even though VR is an interesting approach, there are still many limitations. For instance, the cost of obtaining a VR headset is still unaffordable for universities in developing countries. Therefore it is difficult to have enough devices for everyone to participate and experience chemistry experiments in virtual reality at the same time. Moreover, low-end devices may cause FPS drop and latency while connecting overseas [15] issue in VR. This affects users' vision which causes headaches and dizziness if it is used for a long time.

Another approach also to solve the problem of simulating chemistry experiments is to use augmented reality (AR) [16]. But it seems to lack efficiency for scaling. With the limitations currently available on mobile devices, it is difficult for chemical experiments to be shown with the best precision and clarity.

The above limitations motivate us to develop a chemical experiment simulation on a web platform to overcome the aforementioned barriers and disseminate the simulator to more users. Since the web platform is popular, our system can be run on a computer with an Internet access. This will make the accessibility and everyday practice of users much easier than using VR headsets. In this paper, we introduce the Chemisim simulation system, which provides adequate graphical give a limited computing resource. The laboratory simulation was deployed on a web platform, which allows a wide range of usability for both teachers and students. The simulation is based on real experiments and is supervised by experts in these fields. Fluid simulation is a plus for our system. We analyze and deploy the realistic fluid simulation within an interaction. It is also optimized and can be extracted and uploaded to the web platform. The interaction system is built based on the comments from chemistry teachers and scientists. Each step simulates the actual experiments to provide students with sufficient experience. We also create the 3D laboratory room to be as similar as possible to the real one. In the simulation space, students can look around the room and interact with each item realistically. The step-by-step instruction system allows them to self-learn the subject.

2 PROPOSED FRAMEWORK

2.1 Chemistry Analysis

To maximize the realism of the simulation, we first discussed it with chemistry teachers and scientists. We also visited chemistry laboratories at high schools to specify needed requirements in a real experiment area. We observed the real chemical reaction of different compounded liquids. We also analyzed different results when conducting experiments to reproduce many effects. After that, by following teachers' advice, we develop three particular lessons. The first lesson is an ions recognition assignment using three reagents namely NaCl, Na_2SO_4 and NH_3. The second one is also an ions recognition lesson with KCl, KOH, and K_2CO_3 reagents, but using a centrifuge as a tool. The final lesson specializes in finding advanced chemical substances namely cyclohexene, toluene, hexane and hex-1-in using $AgNO_3$, NH_3 and Br_2 reagents. These lessons are familiar to high school students.

2.2 Fluid Simulation

Fluid simulation is a great challenge in simulating chemistry experiments. First, the color and concentration of chemicals must be very accurate for the user to visualize all the details of a chemical reaction. Second, our development on multi-platform including WebGL [21], in which very limited resources allowed. Note that WebGL is the graphics library for web, which allows almost all Internet browsers to display 3d graphics in real-time. WebGL can be used for virtual reality applications.

Firstly, we create an empty original tube. Inspired by Kronnect [17], we use shader scripts to visualize different colors and the consistency of a liquid. Every liquid is stored in the project as a Unity's prefab [18]. Another challenge is to simulate the process of

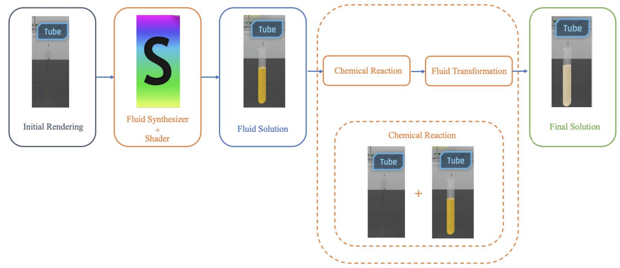

Figure 2: The flow chart of the fluid simulation in our system.

transforming one liquid into another. Changes in color and consistency were consulted by experts and simulated through a chemical state transition system that we developed by changing its shader. Figure 2 shows the flowchart of our liquid simulation component in a chemical reaction.

2.3 Data-driven state machine

For extendability, we propose the data-driven state machine to facilitate the lessons addition in the future. In particular, the system distinguishes each step of a lesson into states. Each state controls the whole lesson with four inter-components, namely, UI Manager, Lesson Manager, Chemical Reaction Manager, and Input Handler.

As seen in Figure 3, the lesson is started with the Instruction State, which shows the introduction on the board. Then, the machine switches to Liquid Taken State, where users can interact with a pipette to get the liquid. After that, Liquid Poured State is selected, where users can use a pipette to pour liquid into the test tube. Each state will control all the components with the required features. For example, in the Liquid Poured State, the state machine uses the UI Manager to display the instruction on the board. Then it controls the lesson manager to initialize the required chemical tubes. The input is allowed by Input Handler for users to drag a chemical tool. The chemical reaction manager runs the respective effects for that experiment. All the logic and constraints are implemented in this state, to stop users from unwanted behaviors. Then it continues until the users complete the lessons when they bypass the Reset State and start again.

We call it "data-driven" since each state is wrapped into a scriptable object, which is a script with data passed in. In that way, with the same behavior, we can clone as many states with different parameters as we want. For example, all the LiquidTaken states from different tubes use the same behavior with different parameters. Instead of creating many scripts to handle different tubes, we pack the LiquidTaken script into a data object with an index, chemical reaction, and message shown as inputs. We refer to these data objects as states. Then, we drag these states to the state machine, where it set each state active sequentially.

The advantage of the data-driven state machine is its extensibility. With a new feature, we simply need to add a new state without refining old scripts. Moreover, with the data wrapped technique, we can reuse each state for different purposes.

2.4 Environment Simulation

The environment simulation consists of four components, namely, laboratory simulation, interactive user interface, web-based deployment and display.

Following discussions with chemistry teachers and scientists, we develop the simulator on Unity engine [18]. We use the Modern Laboratory asset [19] to construct the reality-based laboratory. We used pre-calculated lighting to optimize the performance. We aim to run the application on a web-based platform, thereby maximizing students' opportunities to reach. Due to the incompatibility of the

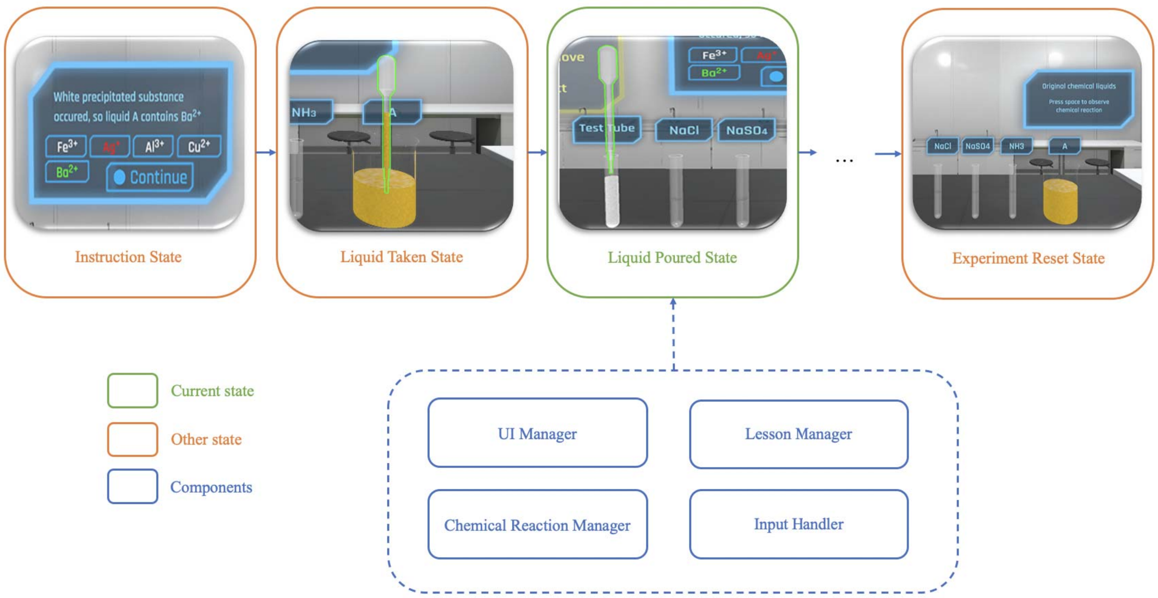

Figure 3: The data-given state machine example including states and components. In the figure, the current state is Liquid Poured State, which controls the liquid pouring feature by using 4 components: UI Manager, Lesson Manager, Chemical Reaction Manager and Input Handler.

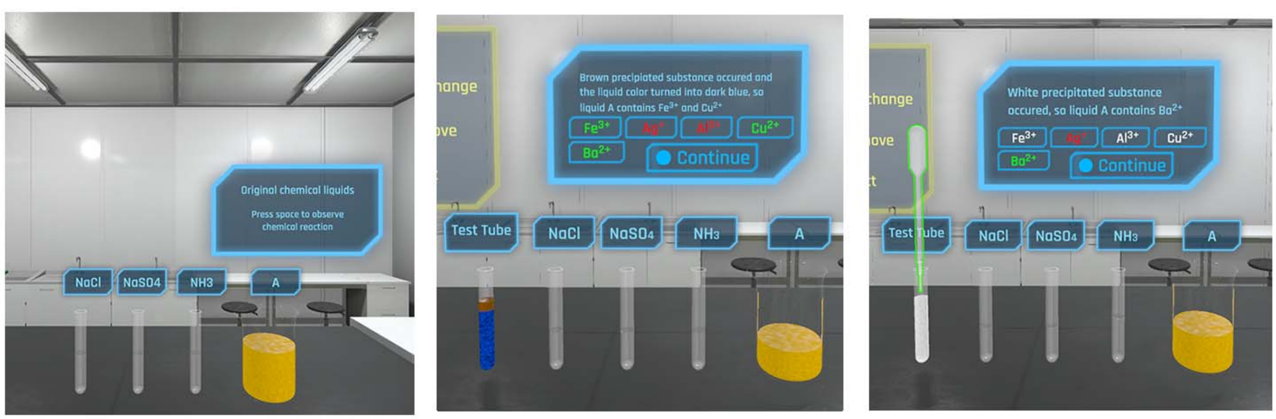

Figure 4: The graphical user interface of the proposed chemical simulator in 3 different versions. From left to right: Basic version - the chemical liquid tubes before and after an experiment are showed, Lite version - the users can observe the chemical reaction step by step, Full version - the users experience the interaction via the laboratory tool and chemical liquids.

laboratory asset, we need to fix shader-related bugs occurring on the Web platform. In particular, we implement unsupported shaders by others as a solution.

For the purpose of simplifying user interactions, we implement the user experience-oriented system. The user interface is embedded into the simulated environment, which is similar to surrounding 3D game objects. Also, it only shows an adequate amount of User Interface elements in each state, thereby users feel comfortable interacting with them. There is an instruction panel near the experiment area, which is used for student guidance.

We deploy the Chemisim simulator on the web platform with three versions, namely basic, lite and full versions. Each version has its respective features as shown in Figure 4. For each version, we modify the graphic quality until it reaches the required frame rate, *i.e.*, 60 fps. Building setting configurations are adjusted for browser compatibility.

In addition, Chemisim also supports the stereoscopic view mode for the immersive Virtual Reality experience on mobile devices, which can be attached to a Google Cardboard [22]. As seen in Figure 5, in each version, we allow users to switch to the Virtual Reality view mode. In that way, users can practice chemistry lessons on Android and iOS devices within the VR experience.

3 Evaluation

To evaluate the simulator, we investigate different versions mentioned earlier, namely, basic, lite, and full versions. The details are as follows.

- Basic Version: Users can only observe the test tubes and press the next button to observe the experiment is performed automatically

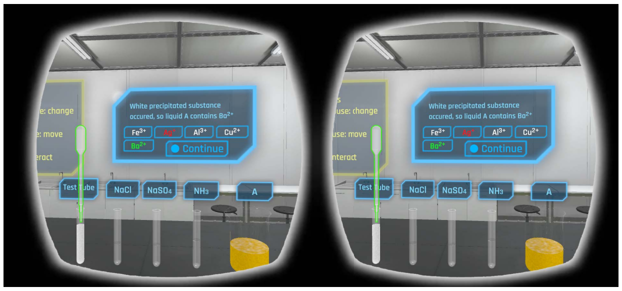

Figure 5: The stereoscopic view mode in Chemisim simulator.

- Lite Version: Users are able to unlock additional features that allow them to move around the lab and observe 3D objects
- Full Version: Users can experience the full features of the simulator including moving freely around the laboratory, interacting and performing experiments with the most realistic reactions.

In total, there are 24 users participating in our user study. We invite users to experience all 3 versions and collect their feedback. All participants have accumulated experience with chemical experiments. They are chemistry students and professors of a university. The male-to-female ratio is 42:58 whereas the average age of the participants is 22.8. Each participant took part in a 30-minute session, namely, a 10-minute trial for each mode. Further, we provide participants with a questionnaire and ask for their feedback. We aim to investigate four following criteria:

- Functionality: Do users feel that the simulator can resolve the problem of simulating chemical reactions?
- Realism: Are chemical reactions similar to those in reality?
- Convenience: Do users feel convenient while using the simulator?
- Preference: How much does the user prefer this version over others?

Since this work focuses on a simulator, the above four factors have great significance for users to choose and use our solution regularly in their learning and working activities.

'Functionality' is the most important criterion of our research. We do not want users to feel that the simulator is just a demo but have to feel they can use it in their real-life activities. As the participants are all experienced in doing chemical experiments, we wanted to check if the color, timing, and interaction in the simulation experiments (Realism) could reach an acceptable level. 'Convenience' and 'Preference' are also important. We anticipate our simulator to be used by many people who now getting into trouble with a lack of chances to do real experiments. Thus our solution needs to offer a convenient, easy to use, and suitable experience for everyone.

The results in Figure 6 indicate that as we gradually unlock more features with each version, users will usually have more positive reactions. Moreover, the full version scores 4+ out of 5 in all criteria. This shows that most users are satisfied with the experience they have when using Virtual Chemistry Lab. However, 4 out of 5 also means that there are many rooms for us to improve. In general, all participants left positive reviews for the idea of the simulator. Most say that colors, chemical names, and interactions in simulated chemical reactions are accurate compared to reality. Some say the simulator still does not have a lot of chemistry experiments to test, but this can be solved with the scalable system we built. This system allows us to create a new chemical reaction in a short period, meeting the needs of the user. Participants also suggest that currently, the initialization of the application is a bit slow. This will affect the first time use experience a lot. The participants also wish to integrate other senses such as taste and smell into the simulator.

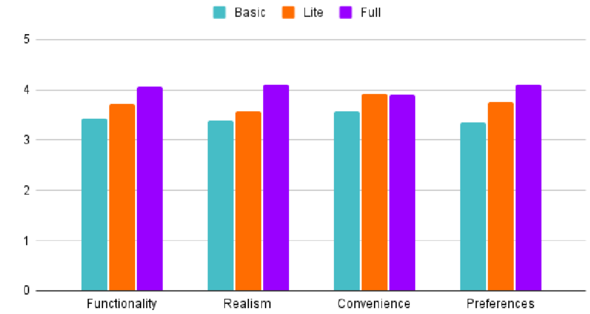

Figure 6: The average rating scores from the user study evaluation for the three modes

4 Conclusion

In this paper, we introduce Chemisim, a web-based VR simulator for chemistry experiments. The simulator supports fluid simulation, the data-driven state machine, and environment simulation. The evaluation via user study shows the usefulness of the proposed simulator in practice. In the future, we plan to extend the simulator for multi-user interaction. For instance, the instructor and students will participate in the same sessions via many devices. In the multi-user mode, the instructor demonstrates the experiments and supervises the students in the virtual environment. We also plan to optimize our simulator for a faster loading.

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